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Cooperative International Science and Engineering Internships

Cooperative International Science and Engineering Internships(CISEI)
Summer 2008 - Student Projects

Student/School	Mentor	Faculty Sponsor	Site Abroad	Student Project
Ricardo Alamillo Chemical Engineering, UCSB	Dr. Brian Peoples	Dr. Raúl Quijada	Departamento de Ingeniería Química y Biotecnología, Universidad de Chile, Santiago Chile	Optimization of synthetic procedures of silice and copper based nanoparticles and the effect of particle size on the physical properties of nanocomposites
Nicholas Anderson Chemistry, University of Washington	Ian Povey	Professor Martyn Pemble	Tyndall National Institute, Cork, Ireland	Atomic Layer Deposition of a Conducting Metal on a Photonic Crystal
Arnaud Berube Physics, University of California, Santa Barbara	Stefan Schulz	Dr. Eoin O'Reilly	Tyndall National Institute, Cork, Ireland	Influence of Polarization Fields on Optical Recombination Rates in GaN-based Quantum Dots
Antoin Douglawi Biochemistry, Allan Hancock College	Manuel Natali	Silvia Giordani	Trinity College Dublin, Ireland	New Materials for Fluorescent Sensing and Imaging
Jennifer Drewes UCSB, Chemistry	Dr. Adriele Prina-Mello and Dr. Aine Whelan	Prof. J. M. Coey and Dr. Yurii Gun'ko	Trinity College, Dublin, Ireland	Functionalization of Metallic Nanowires
Diana Gottschalk Chemistry, James Madison University	Prof. Dongyuan Zhao	Prof. Dongyuan Zhao	Fudan University, Shanghai, China	Design and Synthesis of Zr Supported Mesoporous Catalysts
Madeleine Grossman Chemistry,	Maarten Smulders	Prof. E. W. Meijer	Technical University Eindhoven,	Synthesis and Characterization of Chain Stoppers for Supramolecular

UCSB			Eindhoven, Netherlands	Polymers
<u>Garret Kruger</u> Chemical Engineering, UCSB	Prof. Dongyuan Zhao	Prof. Dongyuan Zhao	Dept of Chemistry and Biochemistry, Fudan University, Shanghai, China	FDU-15 Graphitization using a chromium catalyst
<u>Alison Morrison</u> Chemistry, Santa Barbara City College	Prof. Karin Jacobs	Prof. Karin Jacobs	Experimental Physics, Saarland University, Saarbruecken Germany	Characterization of Nanomaterials: Scanning force microscopy of functionalized surfaces with chemically modified tips
<u>Amanuel Negash</u> Mechanical Engineering, UCSB		Dr. Peter Rogin	Leibniz-Institut für Neue Materialien, Saarbruecken, Germany	Cracking mechanisms in sol-gel silica thin films
<u>Shaun Orr</u> Chemical Engineering, UCSB	Hui Peng	Prof. Andrew Whittaker	Australian Institute for Bioengineering and Nanotechnology, University of Queensland, Australia	Synthesis of Fluorine Containing Polymers for MRI Imaging Agents
<u>Florencia Rusli</u> Chemical Engineering, UCSB	Nicole Grobert	Prof. Andrew Watt	Oxford University, Oxford, England	Alternatives to ITO as a transparent conductor
<u>James Stankowicz</u> Physics, University of Florida	Martin Castell	Martin Castell	Oxford University, Oxford, England	Barium oxide thin films as precursors to barium titanate thin films
<u>Kyle Stewart</u> Electrical Engineering, UCSB	Jaime Muñoz	Luis Vargas	University of Chile, Santiago	Construction of a dc-dc boost converter for an electric car dynamometer
<u>Peter Zalar</u> Chemistry, University of California Santa Barbara	Martin Wolffs	Prof. E. W. Meijer	Eindhoven University of Technology, Eindhoven, Netherlands	Self-assembly of multicomponent porphyrin based systems

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Alamillo's Project Page - CISEI summer 2008



Intern: Ricardo Alamillo, Chemical Engineering, UCSB
Mentor: Dr. Brian Peoples
Faculty Supervisor: Dr. Raúl Quijada
Departamento de Ingeniería Química y Biotecnología,
Universidad de Chile, Santiago Chile

Optimization of synthetic procedures of silice and copper based nanoparticles and the effect of particle size on the physical properties of nanocomposites

Nanocomposites are promising materials as they often have unique properties compared to the filler and matrix material such as enhanced Young's Modulus and permeability. The ability to alter and control the mechanical, optical, and dielectric properties can be advantageous in many applications. Such control in nanocomposite materials may be accomplished by varying the size, shape, and distribution of filler materials in the polymer matrix. Major factors that control the size of the nanospheres (filler) studied are the concentration of surfactant, the temperature of the reaction, and the ratio of water to solvent. In addition it is also important to minimize the size distribution, agglomeration of particles, and if applicable surface oxidation. In this project silica and copper-based nanospheres will be synthesized via sol-gel and reduction processes, respectively, and characterized using x-ray diffraction, scanning electron microscopy, and transmission electron microscopy. The nanoparticles will be added at 0.5-5.0 wt% with respect to the matrix material due to low percolation threshold of nano-sized particulates into the polyethylene and polypropylene (matrix). The physical properties of the modified polymers will be tested and compared to virgin material values. The effect of the addition of silica and copper nanospheres into the matrix will be determined and analyzed. It is hoped that size distribution of nanospheres can control either the Young's Modulus and/or permeability of the nanocomposite.

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Anderson's Project Page - CISEI summer 2008



Intern: Nicholas Anderson, Chemistry, University of Washington

Mentor: Ian Povey

Faculty Supervisor: Martyn Pemble

Advanced Materials and Surfaces, Tyndall National Institute, Cork, Ireland

Atomic Layer Deposition of a Conducting Metal on a Photonic Crystal

Photonic crystals could provide an array of advancements in the fields of photonics and electronics, ranging from photonic gateways in information storage and transfer, to light trapping substances in photovoltaic devices. Integration of photonic crystals into these systems requires a metallic conductive layer. Atomic layer deposition (ALD) offers much promise in depositing thin films of conducting metals onto the porous surfaces of photonic crystals. This project focuses on the growth of copper and iridium on the photonic crystal opal. Preliminary results showed that copper grown by ALD from copper (II) hexafluoroacetylacetonate, $\text{Cu}(\text{hfac})_2$ does not readily grow on silicon, glass, or opal. A self-assembled monolayer (SAM) of octyltrichlorosilane (OCS) was oxidized and employed to seed copper growth on silicon, glass, and titanium oxide grown by chemical vapor deposition (CVD) on glass. Contact angle measurements and infrared spectroscopy proved inadequate at detecting SAM growth. Copper clearly grew on TiO_2 , but was not assisted by the OCS SAM. The SAMs either failed to grow or failed to seed copper growth. Attempts were made at iridium growth on an opal from the precursor, Iridium (III) acetylacetonate, $\text{Ir}(\text{acac})_3$. Visual inspection showed no iridium, though iridium clearly grew in other parts of the ALD kit. Future work will include the use of TiO_2 as a seed layer in copper growth and nitrogen-flow assisted ALD of iridium on opals.

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Berube's Project Page - CISEI summer 2008

Intern: Arnaud Berube, Physics, University of
California, Santa Barbara

Mentor: Stefan Schulz

Faculty Supervisor: Eoin O'Reilly, Photonics Theory
Group, Tyndall National Institute, Cork, Ireland

Influence of Polarization Fields on Optical Recombination Rates in GaN-based Quantum Dots

Due to the wurtzite GaN, conventionally grown GaN-based quantum dots have very high built-in electric fields, which lead to significantly lowered optical recombination rates. We modelled the differences in this conventionally grown GaN-based quantum dot structure versus a newly proposed growth structure for GaN-based quantum dots. We started by using Williams et al.'s solution to the potential of a cuboidal quantum dot structure to model the potential. Then band offsets and effective masses were taken from Suzuki et al. and Vurgaftman and Meyer to model the effective potentials acting on the electron and hole wavefunctions. From here, the finite difference method was used to calculate how these effective potentials affect the solutions to Schrödinger's Equation. And finally, the modulus squared inner product of the electron and hole wavefunctions was used to measure the spatial overlap between the wavefunctions, which is a measure of the optical recombination rates. We found that the newly proposed growth structure for GaN-based quantum dots actually decreased the spatial overlap, decreasing the optical recombination rate

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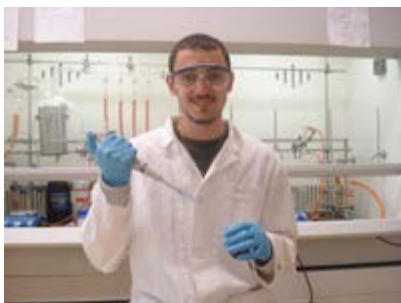
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Douglawi's Project Page - CISEI summer 2008



Intern: Antoin Douglawi, Biochemistry, Allan Hancock College

Mentor: Manuel Natali

Faculty Supervisor: Silvia Giordani

Trinity College Dublin, Ireland

New Materials for Fluorescent Sensing and Imaging

Spiropyrans are photochromic compounds which respond to optical stimulations with significant absorption and emission changes in the visible region of the electromagnetic spectrum. Upon UV irradiation, spiropyrans (SP) adopt the zwitterionic merocyanine form (ME) which produces fluorescence emission; the merocyanine form reverts to the spiropyran upon irradiation with visible light. Spiropyrans bearing a methoxy group in position 8 have been found to exhibit binding abilities with metal ions once in the merocyanine form. This is due to the photogenerated phenolate-methoxy system in the zwitterionic form. In this project we synthesized a new spiropyran bearing a methoxy group in position 8 and a hydroxyethyl chain on the indole nitrogen. We investigated the extent of the abilities of the molecule to bind with various metal ions. We also investigated the effect of different side chains on the behavior of the molecules relating to their absorption. The molecule was selective for Mn, Co, and Zn showing a significant response in the absorption spectra. Other Spiropyran derivatives will be investigated as the project continues along with various types of salts.

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Drewes' Project Page - CISEI summer 2008



Intern: Jennifer Drewes, UCSB, Chemistry
Mentors: Adriele Prina-Mello and Aine Whelan
Faculty Supervisor: Prof. J. M. Coey and Dr. Yurii
Gun'ko
Physics, Trinity College, Dublin, Ireland

Functionalization of Metallic Nanowires

The aim of this project was to bio-functionalize and fully characterize magnetic nickel nanowires to improve their cytotoxicity. It has been previously reported that uncoated Ni nanowires have a time dependent toxic response and it is also well established that biocompatible coatings reduce this toxic response. The biocompatible coatings used for this project were silica and polyethylene glycol (PEG), two well known compounds for nanoparticle surface-coating. The surface-coating was characterized by TEM. Next, nanowires were functionalized with a primary antibody, rabbit anti-mouse IgG. The antibody functionalization was characterized by fluorescence microscopy. After optimizing surface-coating and functionalization procedures, the nanowires were functionalized with secondary antibodies, mouse anti-human, and studies were conducted to look at the cell-functionalized nanowires specific binding.

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Gottschalk's Project Page - CISEI summer 2008



Intern: Diana Gottschalk, Chemistry, James Madison University

Mentor: Prof. Dongyuan Zhao

Faculty Supervisor: Prof. Dongyuan Zhao

Dept of Chemistry and Biochemistry, Fudan University, Shanghai, China

Design and Synthesis of Zr Supported Mesoporous Catalysts

It is already well documented that sulfated zirconia super acids make effective catalysts, specifically in small hydrocarbon isomerization reactions. Superior activity in such reactions is a result of their ability to activate C-C and C-H bonds with Brønsted – Lowery acid sites. In order to maximize the effectiveness of these catalysts the synthesis must be carefully constructed. In this study the ratios of reactants to one another and reaction conditions were varied and the resulting materials characterized using XRD and BET. Variations were made to an already existing experimental procedure that showed the best combination of Zirconia to sulfate was 80%:20% respectively. All work was done using P123 as a scaffold, HCl or H₂SO₄ as acids and ZIPO and tetraethylorthosilicate (TEOS) as precursors. Each catalyst was made in ethanol which was stirring at either 35, 40 or 50C for eight hours. The next day the solvent was evaporated off in an oven at 35C for three days. Finally the catalysts were moved to hotter ovens to crystallize. They were in an 80C oven for 3 days and at last a 100C oven for 12 hrs. The catalysts came out in a fine powder after being scraped off petri dishes and ground in a mortar. It was found that catalysts made with 0.6g P123, 0.5g HCl and at 40C were the most successful.

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Grossman's Project Page - CISEI summer 2008



Intern: Madeleine Grossman, Chemistry, UCSB
Mentor: Maarten Smulders
Faculty Supervisor: Prof. E. W. Meijer
Technical University Eindhoven, Eindhoven,
Netherlands

Synthesis and Characterization of Chain Stoppers for Supramolecular Polymers

For the past decade, supramolecular polymers have emerged as an important class of compounds because they are at the convergence of supramolecular chemistry and materials science. C₃-symmetrical benzene-1,3,5-tricarboxamides (BTAs) are a class of supramolecular polymers that can be considered as a relatively simple model system of particular interest in the study of self-assembly mechanisms and kinetics. Due to intermolecular hydrogen bonding, aromatic interactions and Van der Waals interactions these BTA molecules self-assemble into helical stacks. And studying the self-assembly of a number of BTA molecules has already revealed extensive knowledge about their self-assembly mechanisms. In this study so-called chain stoppers were introduced to the self-assembled stacks of BTAs to inhibit the elongation of the stacks or even to reduce the averaged stack length of these supramolecular polymers, through disruption of the directional non-covalent interactions via specific interactions. Chain stoppers, as well as series of reference compounds not anticipated to inhibit stacking capacity were evaluated through Capillary Viscometry and Circular Dichroism (CD) Spectroscopy measurements. Experimental results indicate the chain stoppers do not function as predicted. No appreciable reduction in CD intensity was observed, indicating chains remain stacked, although it is unclear to what extent. A decrease in viscosity was observed with the addition of chain stopper, however similar changes were observed with the addition of chemically related reference compounds. This suggests that the effect of the chain stopper is not only based upon specific interactions, but is partially the result of less specific interactions, such as changes in solvent polarity. Elucidation of the role of these different interactions and their effect on chain length, using mathematical models to describe the stack growth in the presence or absence of the chain stopper, are anticipated to provide insight into the equilibria governing the self-assembly of the BTA system.

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Kruger's Project Page - CISEI summer 2008



Intern: Garret Kruger, Chemical Engineering, UCSB

Mentor:

Faculty Supervisor: Prof. Dongyuan Zhao,
Dept of Chemistry and Biochemistry, Fudan University,
Shanghai, China

FDU-15 Graphitization using a chromium catalyst

Research has shown that mesoporous (having pores 2-50 nm's) carbon structures can be formed using an Evaporation Induced Self Assembly (EISA) process. Chromium catalyst can adapt this procedure for graphitization which would increase FDU-15's strength and conductivity. This process begins with a Resol precursor, made from phenol, sodium hydroxide and formaldehyde, which provides many hydroxyl groups required for the assembly. Upon mixing Resol with a triblock copolymer (ethylene oxide)₁₀₆-(propylene oxide)₇₀-(ethylene oxide)₁₀₆ (F127) in an ethanol solution the EISA method is initiated. Using F127 with the EISA method produces FDU-15. The steps taken in the EISA method include: ambient evaporation of the ethanol for 5 hours, heating at 100 degrees Celsius for 24 hours and finally carbonizing under nitrogen at 600-1000 degrees Celsius. In this project a chromium catalyst was added during the first step to catalyze graphitization during the final carbonization step. Varying amounts of catalyst and varying carbonization temperatures were studied, in an attempt to create the most graphitic FDU-15 possible. Measurements were taken via XRD and BET to analyze the graphitic character of the sample. At the highest temperature used (1000 C) the samples displayed the best graphitic character; increasing amounts of catalyst did not significantly improve the quality of the graphite. In fact, larger amounts of catalyst resulted in an increase in blocked pores and less surface area. If graphitization is performed at 600 degrees Celsius a larger quantity of catalyst improved the graphitic character.

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Morrison's Project Page - CISEI summer 2008



Intern: Alison Morrison, Chemistry, Santa Barbara City College

Mentor:

Faculty Supervisor: Prof. Karin Jacobs,
Experimental Physics, Saarland University,
Saarbruecken Germany

Characterization of Nanomaterials: Scanning force microscopy of functionalized surfaces with chemically modified tips

abstract

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Negash's Project Page - CISEI summer 2008



Intern: Amanuel Negash, Mechanical Engineering, UCSB

Mentor:

Faculty Supervisor: Dr. Peter Rogin

Leibniz-Institut für Neue Materialien, Saarbruecken, Germany

Cracking mechanisms in sol-gel silica thin films

Sol-gel thin films have wide variety of applications including ceramics coating, anti-reflexive coating of optical instruments, and electronic semiconductor devices. Thin films have the tendency to crack as thickness and temperature is varied. The purpose of this project was to investigate and understand the mechanism involved in the cracking of silicate thin films. Hydrolyzed tetraethyl orthosilicate (TEOS) $\text{Si}(\text{OC}_2\text{H}_5)_4$ was used to create the thin films which were coated on to a standard microscope glass slide substrates. The relationship between film cracking, film thickness and temperature has been researched over the past. In this project we focused on the effects of the adhesion of the film with the substrate on cracking behaviors. Two surface treatments, namely etching with sodium hydroxide (NaOH) and pre-coating with hydroxylapatite (HAP) were used to vary the adhesion strength and improve wetting. In later stage of the experiment, all samples were pre-coated with HAP and the concentration of sodium hydroxide (NaOH) was varied to change the adhesion strength while maintaining a constant film structure. In situ experiments were conducted to capture videos of cracks forming and developing. Our experiment show that substrates with different levels of adhesion strength lead to different types of cracking patterns. The video recordings allowed us to study the kinetics involved. More work is to be done to investigate densification of the silicate thin films.

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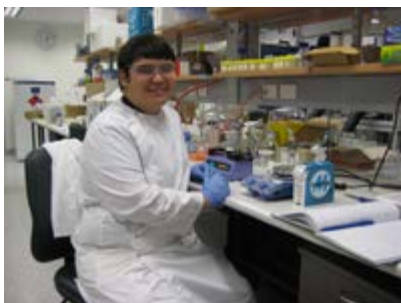
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Orr's Project Page - CISEI summer 2008



Intern: Shaun Orr, Chemical Engineering, UCSB

Mentor: Hui Peng

Faculty Supervisor: Prof. Andrew Whittaker

Australian Institute for Bioengineering and

Nanotechnology, University of Queensland, Australia

Synthesis of Fluorine Containing Polymers for MRI Imaging Agents

Magnetic resonance imaging (MRI), typically used in the medical field, allows for the visualization of the structure and function of various parts of the body. Usually, the hydrogen nucleus is the preferred element used for MRI because of its abundance in the human body. However, any nucleus with a net nuclear spin, such as fluorine-19, can be used for MRI, which is useful to image parts of the body that do not image well using $^1\text{H-NMR}$. The fluorine-containing amphiphilic block copolymers, $p(\text{AA})\text{-}b\text{-}p(\text{nBA-co-TFEMA})$, $p(\text{AA})\text{-}b\text{-}p(\text{TFEMA})$, $p(\text{AA})\text{-}b\text{-}p(\text{AA-co-TFEMA})$, and $p(\text{AA})\text{-}b\text{-}p(\text{AA-co-nBA-co-TFEMA})$ were synthesized for use as MRI imaging agents and micellization was induced to find the relaxation times using $^{19}\text{F-NMR}$. Various techniques were used to characterize the materials, such as GPC, ATR-IR, $^1\text{H-NMR}$, DSC, and DLS. These polymers could possibly be used as MRI contrasting agents.

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Rusli's Project Page - CISEI summer 2008



Intern: Florencia Rusli, Chemical Engineering,
University of California at Santa Barbara

Mentor: Nicole Grobert

Faculty Supervisor: Andrew Watt

Materials, Oxford University, Oxford, England

Alternatives to ITO as a transparent conductor

Indium tin oxide (ITO)'s optical transparency and electrical conductivity makes it an ideal candidate for a transparent conductor in applications such as solar cells and liquid crystal displays. However, indium is in limited supply and the current layer deposition method is costly. Finding a cheaper alternative to ITO is of extreme interest. In this project, carbon-based materials such as graphene and carbon nanotubes (CNTs) were investigated as possible replacements to ITO due to their abundance, production cost, and electrical properties. Graphite flakes were exfoliated through by sonication in organic solvents such as DMF, n-butylamine, THF, and a solution of n-butylamine and THF. CNTs were dispersed by sonication in a solution of n-butylamine and THF. Two methods of film deposition were used: dipping and spraying. The effects of film thickness of graphene and CNTs on conductivity were studied. The resistivity of the films was measured using a four probe method.

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Stankowicz's Project Page - CISEI summer 2008

Intern: James Stankowicz, Physics, University of
Florida

Mentor:

Faculty Supervisor: Dr. Martin Castell
Materials, Oxford University, Oxford, England

Barium oxide thin films as precursors to barium titanate thin films

This project focuses on depositing barium from a getter filament onto an Au(111)-(22 x 3^{1/2}) reconstructed gold surface, and studying the deposited barium with a scanning tunneling microscope. The project is intended to serve as a stepping stone towards the overall goal of creating barium titanate thin films. Barium titanate in bulk has several useful physical properties, and materials with such properties find use in a wide range of devices such as lasers, dynamic random access memory, and transistors. If the properties that make barium titanate useful in bulk can be reproduced in substantially smaller thin film form, any device that uses bulk barium titanate can be reproduced in size by replacing bulk barium titanate with its thin film counterpart. This paper presents background information on thin films, reviews the structures of barium oxide and barium titanate, and covers some of the properties and applications of barium titanate. Work done depositing barium from a getter filament onto a Pt(111) substrate is reviewed, as some of the results were related to and duplicated by the work done here. In this experiment, barium was deposited from a getter filament onto a gold substrate four times, and successfully oxidized three times. By showing that barium can indeed be deposited onto a surface and oxidized, this work paves the way for future work in creating barium titanate thin films on gold surfaces.

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Stewart's Project Page - CISEI summer 2008



Intern: Kyle Stewart, Electrical Engineering, UCSB

Mentor: Jaime Muñoz

Faculty Supervisor: Luis Vargas

FCFM Electrotecnologías, University of Chile, Santiago

Construction of a dc-dc boost converter for an electric car dynamometer

As part of an effort to better understand the capabilities of electric car motors, a project at the Universidad de Chile is to construct a dynamometer. This device can measure the RPM and torque outputs of motors under various conditions, and is being designed for use first with the AERO10, an electric car built at the Universidad, and then to be used with any car. The dynamometer utilizes a separate electric motor as a generator, and this sub-project revolved around building an appropriate high current power converter and resistive load to dissipate that motor's power high power output. At full generative capacity, the motor can output about 200A of current, so heating and current capacity issues are tantamount. The tasks involved included constructing a prototype to test and modify software, reconfiguring a pre-existing high current step-down converter, and implementing adequate safety features due to the extremely high currents being used. The first prototype was of the step-down configuration (buck converter) to help get the actual chopper working again. The second prototype was of the boost converter, and with this the software was modified and proof of concept verified. After extensive modifications, the actual chopper seemed to be working well briefly, but the batteries quickly died and so it is up to the next researcher to continue testing and debugging the high current boost converter. Once the dynamometer is completed, it will also be integrated into a teaching module for electrical engineering students.

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Zalar's Project Page - CISEI summer 2008



Intern: Peter Zalar, Chemistry, University of California Santa Barbara

Mentor: Martin Wolffs

Faculty Supervisor: Prof. E. W. Meijer
Laboratory of Macromolecular and Organic Chemistry,
Eindhoven University of Technology, Eindhoven,
Netherlands

Self-assembly of multicomponent porphyrin based systems

The ability to modify and control the properties of a self-assembled system is one of the most important challenges facing supramolecular chemistry. Molecular positioning, chain length, and reactivity are just some of the properties that are sought to be controlled. Porphyrins are an exciting class of molecules for supramolecular study because they are able to coordinate with metals – giving chemists the ability to functionalize and perform energy transfer studies on the mixed aggregates. The enantiomer of an existing S-chiral porphyrin was synthesized so that “majority rules” and energy transfer experiments could take place in order to give more insight into the interactions between molecules within the aggregates. The R-chiral enantiomer of the existing chiral porphyrin still contains some impurities which are possibly related to the synthetic route taken. The compound will be purified by preparative HPLC. In an attempt to control the size of aggregate stacks, a porphyrin that could act as an endcapper was synthesized and studies were performed to establish the position of the endcapper in the porphyrin system. The techniques used in these experiments included circular dichroism spectroscopy, steady-state photoluminescence, photo luminescent-lifetime, and UV/Vis. These combined studies show that the proposed endcapper molecule is in close proximity to the aggregates. Additional studies need to be performed to establish the endcapper's position in the stack.

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