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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	Department	Student Project
John Aveson Metallurgy and the Science of Materials, University of Oxford, UK	Anand Ramaswamy and Alexander Fang	John Bowers	Department of Electrical and Computer Engineering	Silicon Evanescent Distributed Feedback Lasers
Sei-Won Laura Chang Chemical Engineering, University of Michigan	Nishit Doshi	Samir Mitragotri	Chemical Engineering Department	Polymeric Microparticles of Complex Shapes for Drug Delivery Applications
Qi Chen Chemistry Department of Fudan University, Shanghai, China	Yen-Ping Lin	Luc Jaeger	Chemistry and Biochemistry Department	Exploring the Kinetics of a Hammerhead Ribozyme
Ashley Cooke Theoretical Physics, Trinity College Dublin, Ireland	Michael Villet	Glenn Fredrickson	MRL	Exponential Time Differencing Methods for Stochastic Differential Equations
Yvette Goedegebure Biomedical Engineering, Eindhoven University of Technology, Netherlands	Matthew Black	Matthew Tirrell	Chemical Engineering	Peptide Amphiphiles for Cancer Therapy
Michael Hein Micro- and Nanostructures, Saarland University, Germany	Andrew J. Pascall	Todd Squires	Chemical Engineering	Design of an Induced Charge Electro-Osmosis Microfluidic Pump
Yifan Huang Department of Materials, University of Oxford, UK	Patrick Rinke	Chris van de Walle	Materials	Analytical Calculation of the Auger Recombination Coefficient
Peter Korevaar				Probing Complex

Chemical Engineering and Chemistry, Eindhoven University of Technology, Netherlands	Ravinath Kausik	Songi Han	Chemistry and Biochemistry	Coacervation with Dynamic Nuclear Polarization and Electron Spin Resonance
Björne Mollet Biomedical Engineering, Eindhoven University of Technology, Netherlands	Jos Paulusse	Craig Hawker	MRL	Reversible Supramolecular Polymer Nanoparticles
Donal O'Donoghue Physics, National University of Ireland, Cork	Nathaniel Lynd	Glenn Fredrickson	MRL	Numerical Investigation of the Gyroid Phase of Microphase Separated Block Copolymer Melts Using Self Consistent Mean Field Theory
Ulrike Prüm Chemistry Department, Saarland University, Germany	Alan Kleiman	Eric W. McFarland	Chemical Engineering	Electrocatalysts for Photocatalytic Hydrogen-Production on Fe_2O_3
Yinchao Zhu Chemical Department of Fudan University, China	Hunaid Nulwala	Craig J. Hawker	Materials Research Laboratory	Synthesis and Polymerization of N-Vinyl Triazole Monomers

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Aveson's Project Page - CISEI summer 2008

Intern: John Aveson, Metallurgy and the Science of Materials, University of Oxford, UK
Mentors: Anand Ramaswamy, Alexander Fang
Faculty supervisor: John Bowers
Department: Electrical and Computer Engineering

Silicon Evanescent Distributed Feedback Lasers

Silicon photonics is a rapidly growing field in optoelectronics born out of the desire to produce low cost, high volume optoelectronics devices. These devices are to be compatible with standard complimentary metal-oxide-semiconductor (CMOS) processing technologies that will then allow the seamless integration of electronics and photonics on a single material platform. Silicon has an indirect band gap of 1.1eV, corresponding to ~1100nm which is not a standard communication wavelength. Additionally it does not demonstrate an electro-optic effect owing to its cubic crystal structure which requires the development of novel methods for signal modulation. However, these problems have been circumvented by the hybrid silicon platform [1], which has been used to produce optical devices that operate in the standard telecommunication windows of 1310nm and 1550 nm. This enables the use of the devices in fibre optic systems, such as in data transfer in high speed computing. In the case of the silicon evanescent laser, a waveguide is etched onto a silicon-on-insulator (SOI) substrate, and the evanescent tail of the optical mode in the waveguide is amplified in a InAlGaAs multiple quantum well region bonded to the silicon wafer. In this study, threshold current, maximum power output and differential efficiencies are obtained for novel distributed feedback (DFB) lasers and are correlated to the design parameters. Emission spectra are obtained using an optical signal analyser. Small signal modulation at radio frequencies is carried out to indicate device performance in data transfer applications.

[1] AW Fang, H Park, YH Kuo, R Jones, O Cohen, D Liang, O Raday, MN Sysak, MJ Paniccia, JE Bowers, Materials Today 10 (2007) 28-35

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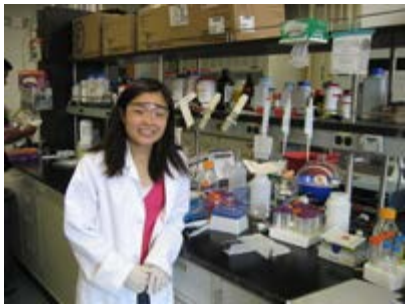
Chang's Project Page - CISEI summer 2008



Intern: Sei-Won Laura Chang, Chemical Engineering, University of Michigan
Mentor: Nishit Doshi
Faculty supervisor: Samir Mitragotri
Department: Chemical Engineering

Polymeric Microparticles of Complex Shapes for Drug Delivery Applications

Polymeric micro- and nanoparticles are useful in many applications including drug delivery and medical imaging. Various improvements have been made to polymeric particles in order to enhance the specificity and efficiency of particles within the body. The surfaces of biphasic particles, particles made of two different polymers, can be specifically modified with biomolecules. Moreover, imaging agents such as magnetite or quantum dots can be incorporated in particles for diagnostic work. Thus far, these complex particles have been limited to a spherical shape. Particle shape plays a critical role in the particle performance in the body, affecting parameters including targeting efficiency, particle degradation and phagocytosis. In this study, a custom film stretching technique [1] is used to manipulate the shape of spherical biphasic and magnetic microparticles. Rod-shaped particles are made using spherical biphasic poly(lactic-co-glycolic acid) microparticles and spherical paramagnetic microparticles as a starting point. Future work involves quantifying the physical characteristics of these particles. Thus, another degree of complexity has been added to polymeric particles which have wide applications in biomedicine.

[1] Champion, J. et al. 2007.

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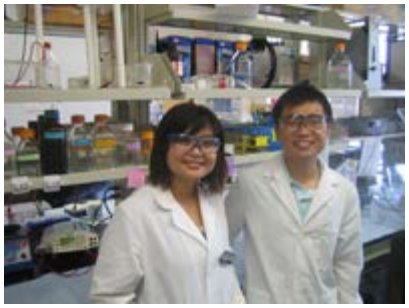
Chen's Project Page - CISEI summer 2008



Intern: Qi Chen, Chemistry Department of Fudan University, Shanghai, China
Mentor: Yen-ping Lin
Faculty supervisor: Luc Jaeger
Department: Chemistry and Biochemistry

Exploring the Kinetics of a Hammerhead Ribozyme

This program focuses on the kinetics of Hammerhead Ribozyme, a RNA enzyme. The reaction we worked on is the trans-cleavage of a RNA substrate on the enzyme, and our focus is on how the loop-loop interaction could affect the catalyzing process. Therefore, we designed a series of similar enzymes through nucleotide mutations to vary the strength of the loop-loop interactions. By labeling the substrates with radioactive phosphorus isotope, so that we can measure the concentrations of the product and the remaining reactants and by controlling the reactions times accurately, the kinetic rate constants of each reaction can be obtained. We compared the kinetic rate constants of the different reactions and made the conclusion that the loop-loop interaction enhances the catalyzing effect of Hammerhead Ribozyme. This research gives us more information about Hammerhead Ribozyme, so that hopefully in the future we can use this RNA enzyme to form cages of different shapes as a carrier of drugs for genetic therapy.

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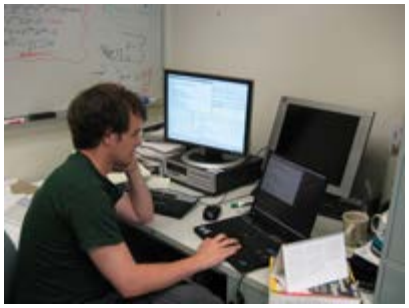
Cooke's Project Page - CISEI summer 2008



Intern: Ashley Cooke, Theoretical Physics, University of Dublin, Trinity College, Ireland
Mentor: Michael Villet
Faculty supervisor: Glenn Fredrickson
Department: Materials Research Laboratory

Exponential Time Differencing Methods for Stochastic Differential Equations

Field theoretic models coupled with the mean field approximation are a powerful tool in investigating the equilibrium behavior of polymeric fluids. However, in some physical systems, such as polyelectrolytes, the mean field approximation is insufficient to properly capture the physics of the system. To explore beyond-mean-field physics we use the complex Langevin technique, which involves the solution of a set of non-linear stochastic differential equations, to simulate field theoretic fluid models of polymers. We wish to develop algorithms to solve these equations with good stability and high order of (weak) accuracy to increase efficiency of our simulations. Exponential differencing (ED) schemes have been developed with high stability and order of accuracy for partial differential equations, and we aim to adapt these methods for the stochastic case with the hope of preserving these desirable properties. The test system for our algorithms consists of a one-dimensional non-linear Langevin equation with a Gaussian noise term. We develop several ED algorithms and compare their performance in simulating the test system against established methods such as the Euler-Maruyama and Petersen-Öttinger schemes (E.M. Lennon et al, 2008).

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Goedegebure's Project Page - CISEI summer 2008

Intern: Yvette Goedegebure, Biomedical Engineering, Eindhoven University of Technology, Netherlands
Mentor: Matthew Black
Faculty supervisor: Matthew Tirrell
Department: Chemical Engineering

Peptide Amphiphiles for Cancer Therapy

Research has shown that the antimicrobial peptide sequence KLAKLAK KLAKLAK (KLA) is nontoxic to eukaryotic cells. However, once KLA enters the eukaryotic cell it becomes cytotoxic and disrupts the negatively-charged mitochondrial membrane. As a consequence, cytochrome c is released and triggers apoptosis (death) of the cell. When a hydrophobic carbon tail is attached to the hydrophilic KLA peptide, a peptide amphiphile is formed. Past research has shown that the concentration needed to kill 50 % of the cells (IC50) is almost two orders of magnitude lower when a KLA peptide amphiphile with a C12 carbon tail is used. The hydrophobic tail may improve the cell uptake by associating the peptide more strongly with the membrane and making KLA more resistant to protease digestion. This research will study the effects of the hydrophobic tail length and investigate if an optimum length can be found. Experiments with liposomes that mimic different membranes will be conducted to help analyze how the peptide amphiphile disrupts the membrane. In order to investigate the mechanism, circular dichroism, dynamic light scattering and liposome leakage experiments will be used. The difference in the IC50 for various tail lengths will be tested on different tumor cell lines. Ultimately the peptide amphiphile may be used as part of a mixed micelle to treat cancer by causing apoptosis of the cells.

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Hein's Project Page - CISEI summer 2008

Intern: Michael Hein, Micro- and Nanostructures, Saarland University, Germany
Mentor: Andrew J. Pascall
Faculty supervisor: Todd Squires
Department: Chemical Engineering

Design of an Induced Charge Electro-Osmosis Microfluidic Pump

In recent years so called “lab-on-a-chip” devices have gained more importance. One of the last hurdles to overcome with regard to in-field deployment is the lack of a miniaturized pressure source. Induced Charge Electro-Osmosis (ICEO) offers one possible solution to that problem. The main advantage of ICEO compared to classical electrokinetics is that the potential driving the flow is applied perpendicularly. This results in a much closer spacing between the electrodes and thus leads to higher field strength for the same voltage. High pressures on the order of magnitude of several atmospheres could be realized using a battery as a power source. This project dealt with the design of a pump based on a packed bed of hemispherically metallized microbeads located in a pump chamber. When the field is applied, ICEO forces the fluid to flow toward the metallic side of every bead. A packed bed of oriented beads in a sealed chamber will induce a net flow that must be equalized by a back flow. Since the pores between beads are in the micron range, a very large pressure is built up.
To produce the pump, microbeads were spin coated on a wafer, metallized and later transferred into the device made out of Polydimethylsiloxane (PDMS). The packed bed of beads is an essential part of the pump and was formed using either gravitational settling or centrifugal forces to orient the metallized beads. The effectiveness of different designs will be studied using various techniques.

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Huang's Project Page - CISEI summer 2008

Intern: Yifan Huang, Department of Materials, University of Oxford, UK
Mentor: Patrick Rinke
Faculty supervisor: Chris Van de Walle
Department: Materials

Analytical Calculation of the Auger Recombination Coefficient

Light emitting and laser diodes (LEDs and LDs) in the green to ultraviolet part of the spectrum are based on Indium-Gallium nitride (InGaN) alloys as the active light-emitting region. To increase the cost effectiveness, and to open up applications for solid state lighting, an increase in Internal Quantum Efficiency (IQE) is required. The IQE of InGaN devices is currently limited by severe loss mechanisms that, at high driving currents (i.e. high free carrier concentrations), actually lead to a decrease in IQE and light output . Recently Auger recombination has been proposed as a loss mechanism under typical operating conditions of InGaN devices. This process scales with the cubic power of the free-carrier concentration and would thus dominate at the observed reduction in IQE. However, calculating the Auger rate from first principles is difficult and demanding involving integration in eight dimensions. Here we present an analytical derivation of the Auger rate following earlier work by Haug et al. (1978), but for a different Auger process. For the derivation we assume energy bands to be parabolic and isotropic and the matrix elements, which describe the inter-electronic interaction as a constant taken from first principle calculations performed in the group. The resulting expression for the Auger coefficient enables not only a better understanding of its analytical dependence on materials parameters (which can often be hard to deduce otherwise), but also provides an important crosscheck for a fully numerical solution of the Auger rate that is undertaken independently.

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Korevaar's Project Page - CISEI summer 2008

Intern: Peter Korevaar, Chemical Engineering and Chemistry, Eindhoven University of Technology, Netherlands
Mentor: Ravinath Kausik
Faculty supervisor: Songi Han
Department: Chemistry and Biochemistry

Probing Complex Coacervation with Dynamic Nuclear Polarization and Electron Spin Resonance

Complex coacervation is a liquid-liquid phase separation due to the interaction between different charged colloids, polycations and polyanions. Under specific pH conditions, these colloids coalesce, yielding a higher and a lower concentrated phase in the colloidal component. This form of polymer complexation has great potential to be applied in food technology, build-up of new materials, or as blended polymers for e.g. drug delivery. In order to better utilize complex coacervation in material science applications, an in depth understanding of the structure and dynamics of this complexation process is important. Therefore, polycation polyvinylimidazole was functionalized with a 2,2,6,6-tetramethylpiperidinyl-1-oxyl (TEMPO) spin probe and coacervated with polyanions alginate and polyaspartic acid. The nitroxide free radical in the spin probe enables us to measure Electron Spin Resonance (ESR) and Dynamic Nuclear Polarization (DNP) on coacervation. The rotational chain mobility of the spin probe bearing polymer can be determined from fitting of the ESR spectra, while the hyperfine splitting due to the presence of a nitrogen atom reveals the polarity close to the spin probe. The translational dynamics of the solvent close to the spin probe was determined from the DNP enhancements, caused by the dipolar coupling between spin probe and 1H in water.

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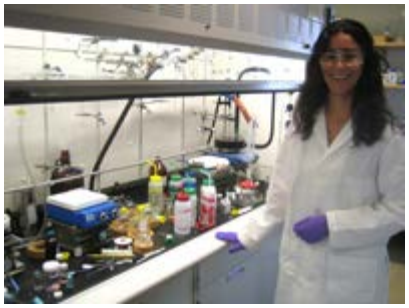
Mollet's Project Page - CISEI summer 2008



Intern: Björne Mollet, Biomedical Engineering, Eindhoven University of Technology, Netherlands
Mentor: Jos Paulusse
Faculty supervisor: Craig Hawker
Department: Material Research Laboratory

Reversible Supramolecular Polymer Nanoparticles

In this project, reversible nanoparticles are produced by intramolecular crosslinking of organic polymers. The reactive side-groups that are responsible for the crosslinking are based on the ureidopyrimidinone (UPy) moiety which consists of four hydrogen bonding units that can dimerize. Since the UPy crosslink is non-covalent, a polymer chain functionalized with UPy side-groups can fold itself into an energetically stable state: a nanoparticle. Although this process deals with completely synthetic molecules, it is believed it can be useful as a simplified model to gain a better understanding in the complex processes of protein folding. In addition, since the UPy crosslink is reversible, the polymer nanoparticles will have a reversible nature. Once the nanoparticles are triggered to open up, the polymers can react intermolecularly with each other, resulting in the formation of crosslinked networks. These properties may make the nanoparticles suitable for a wide variety of applications, from nanomedicine to rheological switch.
The polymers are characterized by nuclear magnetic resonance and gel permeation chromatography. Infrared spectroscopy is used to follow the functionalization of the polymers with UPy side-groups via urea bonds. Dynamic light scattering and viscometry are used to indicate the formation and stability of the nanoparticles. After studying the biocompatibility of the nanoparticles, future work may include adding drugs or imaging agents to these nanoparticles, making them suitable for a variety of biomedical applications.

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O'Donoghue's Project Page - CISEI summer 2008

Intern: Donal O'Donoghue, Physics, National University of Ireland, Cork
Mentor: Nathaniel Lynd
Faculty supervisor: Glenn Fredrickson
Department: Materials Research Laboratory

Numerical Investigation of the Gyroid Phase of Microphase Separated Block Copolymer Melts Using Self Consistent Mean Field Theory

Silicon photonics is a rapidly growing field in optoelectronics born out of the desire to produce low cost, Using self-consistent mean field theory, we investigate the equilibrium phase behavior of A(AB)3 miktoarm-star triblock copolymers. Immiscibility of the constituent A- and B-blocks of these copolymers leads to phase separation on the nanometer length-scale into ordered morphologies. By varying the relative composition and interaction strength between the different covalently-bound species in our model, we can numerically investigate block copolymer phase behavior. Specifically, we seek portions of the phase diagram in which the gyroid structure (Ia3d, space group 230) is the equilibrium morphology, by identifying the transitions from the gyroid morphology to the lamellar, and to the hexagonally packed cylindrical morphologies.

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Prüm's Project Page - CISEI summer 2008

Intern: Ulrike Prüm, Chemistry Department, Saarland University, Germany
Mentor: Alan Kleiman
Faculty supervisor: Eric W. McFarland
Department: Chemical Engineering

Electrocatalysts for Photocatalytic Hydrogen-Production on Fe_2O_3

This study aims to find an appropriate electrocatalyst for the oxygen evolution reaction (OER) on an a-Fe_2O_3 (hematite) semiconducting solar absorber that decreases the overpotential for the OER for water oxidation. The OER is the rate determining step for water splitting on bare hematite photo-electrodes, limiting the overall efficiency of hydrogen production. Hematite is electrodeposited on fluorine-doped tin oxide substrates and electrocatalyst candidates including RuO_2 and Ni-based alloys are deposited on the substrates by electrodeposition and spray pyrolysis. The activity for OER is quantified by analysis of the current-voltage relationship of the electrode substrate, with RuO_2 and Ni-50wt% Cu demonstrating the best electrocatalytic performance. Additionally the competition between the hydrogen evolving reaction (HER) and the oxygen reduction reaction (ORR) at the cathode is investigated. Since the oxygen produced at the anode remains partly in solution, it is important to find a cathode-material that favors the HER. The effect of the presence oxygen on different metals as cathodes is tested with cyclic voltammetry in gas-saturated solutions. Oxidation saturates surface sites allowing the HER to be maximized compared to the ORR; W and Mo show extensive surface oxidation, whilst for Pt and Ag it is minimal.

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Zhu's Project Page - CISEI summer 2008

Intern: Yinchao Zhu, Chemical Department of Fudan University, China
Mentor: Hunaid Nulwala
Faculty supervisor: Craig J. Hawker
Department: Materials Research Laboratory

Synthesis and Polymerization of N-Vinyl Triazole Monomers

The goal of this project is to synthesize and polymerize N-vinyl triazole monomers and evaluate their properties. Triazoles are chemically and thermally stable aromatic compounds with hetero atoms capable of hydrogen bonding [1], which suggest some potential applications in the fields of biochemical, medical, pharmaceutical, and membrane materials. So we want to further investigate properties of triazoles and their effect on polymeric materials. The synthesis of the high yielding triazole monomers is based on the Cu catalyzed 'click' reaction between an alkyne and the azides, which requires benign reaction conditions[2]. Currently, library of N-vinyl triazole based materials such as 4-(trimethylsilyl)-1-vinyl-1,2,3-triazole, 4-phenyl-1-vinyl-1,2,3-triazole, and tert-butyl (1-vinyl-1,2,3-triazol-4-yl)methylcarbamate, is synthesized and being purified. And we have synthesized and purified a chain transfer agent (CTA), [1-(O-Ethylxanthyl)ethyl] benzene[3] for future work. In the near future, we will polymerize these monomers by employing living-radical polymerization methods based on chain transfer agents (CTA). Chemical and thermal properties of those materials are to be subsequently analyzed using DSC (differential scanning calorimetry), TGA (thermo gravimetric analyzer) and GPC (gel permeation chromatography) techniques.

[1] Heterocyclic chemistry T.L. Gilchrist ISBN 0-582-01421-2
[2] V. V. Rostovtsev, L. G. Green, V. V. Fokin, K. B. Sharpless, Angew. Chem., 2002, 114, 2708-2711
[3] Decheng Wan,† Kotaro Satoh,† Masami Kamigaito,*,† and Yoshio Okamoto‡, Macromolecules 2005, 38, 10397-10405

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