MATERIALS RESEARCH LABORATORY at UCSB: an NSF MRSEC

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Cooperative International Science and Engineering Internships

Cooperative International Science and Engineering Internships(CISEI)
Summer 2009 - Student Projects

Student/School	Mentor	Faculty Sponsor	Department	Student Project
Dirk W. R. Balkenende Chemical Engineering and Chemistry, Eindhoven University of Technology, Netherland	Dan Burke and Elizabeth Amir	Craig Hawker	Materials Research Laboratory	Synthesis of Accessible N-Type Organic (Opto)Electronic Polymers
Jenny Butler Chemistry and Forensic Department, University College Cork, Ireland	Rahau Shirazi	Cyrus Safinya	Materials Research Laboratory	Characterisation of Degradable Cationic Lipids for Gene Delivery
Yue Cai Chemistry Department of Fudan University, Shanghai, China	Yichi Zhang	Galen D. Stucky	Chemistry and Biochemistry Department	Preparation of Metal Doped Mesoporous TiO_2 Sub Microspheres and Application in Dye Degradation
Luke Gordon Theoretical Physics, Trinity College Dublin, Ireland	Maosheng Miao	Chris Van de Walle	Materials Department	Simulation of 2-Dimensional Electron Gas in Algan/Gan High Electron Mobility Transistors
Shane Heffernan Advanced Materials Trinity College Dublin, Ireland	Jun Lin	Omar Saleh	Materials Research Laboratory	Stress Fields in Microtubule Networks
Almuth Hoffmann Physics, Saarland University, Germany	Andrew J. Pascall	Todd Squires	Chemical Engineering	Induced Charge Electroosmosis over Self-Assembled-Monolayers
Jodie Melbourne Materials Science, University of Oxford, UK	Nathaniel Lynd	Craig Hawker and Jean Marie Tarascon	Materials Research Laboratory	Nanostructured Li-Polymer Electrolytes
Luuk Olijve Biomedical Engineering,	Ravinath Kausik		Chemistry	The Effect of Cholesterol on

Eindhoven University of Technology, Netherlands	and Sunyia Hussain	Songi Han	and Biochemistry	Phospholipid Bilayers Studied by DNP Enhanced ^{1}H NMR
Brian Rochford Mathematics, University College Cork, Ireland	Robert Hoy	Glenn Fredrickson	Materials Research Laboratory	Reversible Simulations of Associating Polymers
Stefan Schommer Materials Science, Saarland University, Germany	Yanli Gong	Gary Leal	Chemical Engineering	Effects of Reactive Compatibilizer on Immiscible Polymer Blends
Min Tang Chemistry, Fudan University, China	Joshua D. Furman	Anthony K. Cheetham	Materials Research Laboratory	Anthroquinone Luminescence in Inorganic-Organic Hybrid Framework Materials

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Balkenende's Project Page - CISEI summer 2009

Intern: Dirk W. R. Balkenende, Chemical Engineering and Chemistry, Eindhoven University of Technology
Mentors: Dan Burke, Elizabeth Amir
Faculty supervisor: Craig Hawker
Department: Materials Research Laboratory

Synthesis of Accessible N-Type Organic (Opto)Electronic Polymers

Semiconductors based on organic polymers are excellent alternatives to silicon based semiconductors for a wide variety of applications. Alluring characteristics of organic semiconductors include flexibility, low costs, ease in processing, and color tunable light emission. A large amount of research in organic electronics is focused on oligo- and polythiophenes (OTs and PTs) and their derivatives. Until recently mainly p-type polymers were developed, while PTs derivatives can potentially exhibit n-type behavior. To obtain efficient n-type polymers it is crucial to decrease the HOMO-LUMO energy gap and improve material ordering. One way to tune electronic properties from p- to n-type is by introducing electron withdrawing groups into the polythiophene skeleton. It was shown in the past that oxygenation of sulfur atoms in the OTs into the corresponding S,S-dioxides can lead to a lowering of the HOMO-LUMO energy gap, and lead to the highly ordered molecular chains. The first project will focus on fully oxygenating thiophene polymers with the use of the very strong oxidizing agent HOFÌCH_3CN, and possibly observe n-type behavior. The second project will focus on synthesizing selenophene based monomers. We plan to study the oxidation of these monomers with the HOFÌCH3CN and further use them to construct selenophene based polymers. We also plan to examine the electronic properties of the polymers as active layers in electronic devices.

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Butler's Project Page - CISEI summer 2009

Intern: Jenny Butler, Chemistry and Forensic Department, University College Cork
Mentor: Rahau Shirazi
Faculty supervisor: Cyrus Safinya
Department: Materials Research Laboratory

Characterisation of Degradable Cationic Lipids for Gene Delivery

The future of gene therapy using non-viral vectors such as cationic lipids (CL) requires in depth understanding of the obstacles such as low transfection efficiencies (TE) and cytotoxicity of CL. A series of newly synthesized cationic multivalent lipids ($CMVL_n$) where (n= +2, +3, +4, +5) have been designed to address the above barriers. CMVLn contains a degradable spacer expected to degrade in the reducing environment of the cytoplasm by glutathione (GSH). For transfection purposes, the CL needs to efficiently condense DNA molecules. In this study, the ability of the $CMVL_n$s to condense DNA and GSH effect are measured using the Ethidium Bromide (EtBr) displacement assay. EtBr fluoresces once intercalated between the DNA base pairs but that fluorescence is quenched when a CL-DNA complex forms. EtBr self quenches in the solution hence the fluorescence decrease. The results show that $CMVL_n$s are capable of condensing DNA and the addition of GSH prevents the complex formation via lipid degradation for the $CMVL_n$s. The addition of GSH to corresponding CLs with no degradable bond had no effect on the CL-DNA complex formation indicating that GSH effect is highly specific to CMVLns. We are continuing to study the cytotoxicity effect of the $CMVL_n$s as compared to the corresponding CL with no degradable bond. The result shows lower cytotoxicity for the $CMVL_n$s. These degradable CL-vectors open the way for the development of efficient non toxic CL-vectors.

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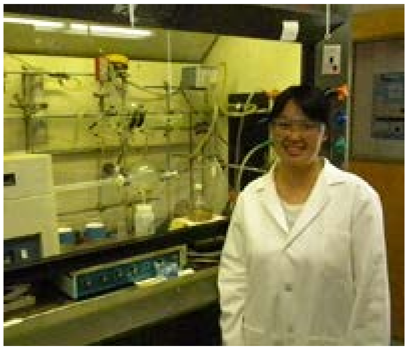
Cai's Project Page - CISEI summer 2009



Intern: Yue Cai, Chemistry, Fudan University
Mentor: Yichi Zhang
Faculty supervisor: Galen D. Stucky
Department: Department of Chemistry and Biochemistry

Preparation of Metal Doped Mesoporous TiO_2 Sub Microspheres and Application in Dye Degradation

TiO_2 is one of the most popular photo catalysts used in photo-catalytic oxidation of wastewater treatment due to its chemical inertness, low costs, and non-toxicity. But its application in organic compound degradation is limited to UV light. Metal doped TiO_2 shows improved photo-catalytic activity under visible light. We prepared Fe and Cu doped mesoporous TiO_2 microspheres via aerosol-spray. This technique allows for continuous, relatively easy, large-scale production of nanoparticle materials. The composition, morphology and porous structure of the sphere can be easily controlled via reaction conditions. It is one of a few well-developed methods for synthesizing high-surface-area meso-structures with diverse metal oxide components. TEM was used to reveal the mesoporous sphere morphology along with SEM, EDX, and UV-Vis for further characterization of the products. XRD pattern indicated a pure anantase crystal phase of TiO_2. BET results suggested the meso-pores have very uniform sizes. As an application, we tested the dye degradation to show the high activity of the materials as made, especially under visible light irradiation. Photo-catalytic activity of the spheres was tested in a methyl red degradation reaction. Results showed enhanced photo-catalytic activity for the doped spheres with respect to the absence of them under visible light. We hope these metal-doped spheres can be applied to environmental, biological, and chemical fields as catalysts in industrial scale reactions.

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Gordon's Project Page - CISEI summer 2009

Intern: Luke Gordon, Theoretical Physics, University of Dublin, Trinity College
Mentor: Maosheng Miao
Faculty supervisor: Chris Van de Walle
Department: Materials Department

Simulation of 2-Dimensional Electron Gas in Algan/Gan High Electron Mobility Transistors

AlGaN/GaN high electron mobility transistors (HEMTs) have been intensively studied due to their applications in high power and high frequency devices. Several problems hinder the improvement of the device performance including most notably the origin of the two-dimensional electron gas (2DEG). Our recent first principles calculations showed high level AlGaN surface states that might be the source of the 2DEG[1]; however, it is unclear how the surface features can alter the density and mobility of the 2DEG. Recent experiments observed that the surface barrier height continuously increases with the AlGaN thickness[2]. In this work, we examine the relation between surface state distribution and the 2DEG density by implementing the surface state with finite and distributed density into a Schrodinger-Poisson simulator, nextnano3[3]. Using the new program, the 2DEG density change with a changing surface barrier height is simulated and compared with experimental results for several different compositions of AlGaN. It is shown that the change in surface barrier height is highly dependent on the composition as well as the surface qualities of the material. In addition, the 2DEG density of N-polar HEMTs and their dependence on the doping level and profile as well as on the surface state level are simulated and compared with recent experiments[4].

[1] M. S. Miao, J. Weber, C. G. Van de Walle, to be submitted.
[2] S. Chowdhury, M. Higashiwaki, M. S. Miao2, B. L. Swenson1, C. G. Van de Walle, and U. K. Mishra, submitted to 36th International Symposium on Compound Semiconductors (ISCS-2009)
[3] http://www.nextnano.de/nextnano3/
[4] M. H. Wong, Y. Pei, J. S. Speck, and U. K. Mishra, Appl. Phys. Lett. 94, 182103 (2009).

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Heffernan's Project Page - CISEI summer 2009

Intern: Shane Heffernan, Advanced Materials Trinity College Dublin
Mentors: Jun Lin and Megan Valentine
Faculty supervisor: Omar Saleh
Department: Materials Research Lab

Stress Fields in Microtubule Networks

A bottom up approach to studying the behaviour of the cell cytoskeleton is taken by attempting to find the mechanical properties of reconstituted microtubule networks. Such networks, formed from the polymerisation of alpha-beta tubulin dimers, appear capable of reorganising themselves in order to carry out critical cell functions. An understanding of their basic mechanical properties is a necessary basis for modelling this biological behaviour. Magnetic bead microrheometry (MBMR) is developed as a novel means of probing the stress moduli such weak, viscoelastic networks using water based polyacrylamide (PAAm) gels. Both magnetic and non-magnetic beads are embedded within the network during the polymerisation before gelation occurs. The data space for Youngs' modulus was estimated to be 10^{-2} – 10 Pa. PAAm gels at 2.9% (w/w) AAm 1:80 AAm:cross-linker ratio and 3% AAm 1:90 AAm: cross-linker were found to possess viscoelastic properties. A partial liquid- solid gel phase space based on varying AAm and crosslinker concentration provides motivation for more complete research into monomer and cross-linker concentration dependence of PAAm gels.
Qualitative tests using MBMR on taxol-stabilised microtubule networks under stresses ranging from 20-31pN verified characteristics not common to all gels. At 4.5% (w/v) tubulin concentration, plastic deformation is observed with an elastic limit of 4-5ìm. Local network failure under 31 pN forces was observed. Anisotropic network deformation without long range order, identified from offsets of up to 50^{o} of the magnetic bead deformation with respect to applied force, was observed in all samples. Microtubule networks with 1:25 biotin labelled tubulin cross-linked with streptavidin in marginal excess of this ratio exhibited a 10^{2} increase in stress moduli. These results provide a basis for developing more quantitative measurements and probing stress moduli dependence on microtubule, taxol and cross-linker concentration.

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Hoffmann's Project Page - CISEI summer 2009

Intern: Almuth Hoffmann, Physics, University of Saarland
Mentor: Andy Pascall
Faculty supervisor: Todd Squires
Department: Department of Chemical Engineering

Induced Charge Electroosmosis over Self-Assembled-Monolayers

With increasing interest in microfluidic devices, such as portable "labs-on-a-chip", the question arises how to pump and mix fluids in microchannels. A new phenomenon, induced charge electroosmosis (ICEO) promises to provide low voltage and high pressure fluid pumping integrated on-chip. This nonlinear electroosmotic flow results from the interaction between the electric field and the polarisable surface by inducing a diffuse layer of charge (double-layer) near the surface. This layer is then forced to move by the applied field. Since the field induces and drives the double-layer, the flow scales like E^2. Thus, AC fields can be used avoiding electrochemical reactions that plague standard electroosmosis. Also the flow is perpendicular to the applied field, so lower voltages are needed.
The recent experiments have shown 10 to 1000 times slower slip velocities than expected by standard theory (Bazant, et al., 2009); we examine the hypothesis that the surface is contaminated by unknown substances. We use the well-known gold-thiol interaction to generate self-assembled-monolayers (SAMs) with thicknesses between 0.4nm and 2.4nm to model adventitious surface contamination. Theory suggests that the velocity will be reduced by a factor of $(1+\varepsilon_w d/\varepsilon_d \lambda)^{-1}$, where ε_w/λ and ε_d/d are the capacitances of the double-layer and contaminant-layer respectively. As expected, the velocity is about 100 times smaller than standard theory.
But considering the SAM-effect, we see significantly better qualitative agreement. However, accordance over a large range of parameters is still missing. This suggests that important physics are still missing from our model. Future work will concentrate on determining this physics.

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Melbourne's Project Page - CISEI summer 2009

Intern: Jodie Melbourne, Materials Science, University of Oxford
Mentor: Nathaniel Lynd
Faculty supervisor: Craig Hawker and Jean Marie Tarascon
Department: Materials Research Laboratory

Nanostructured Li-Polymer Electrolytes

Current Lithium-ion batteries contain electrolytes that are both flammable and toxic. The use of a solid block copolymer based electrolyte mitigates these problems. A block copolymer is made up of covalently-bound blocks of different polymers, in our case poly(styrene)-b-poly(ethylene oxide), PS-PEO. Microphase-separation arises in PS-PEO due to the incompatibility between the PS and PEO blocks, with structures depending on the relative amounts of the two components. Unfortunately, solid block copolymer electrolytes only exhibit ionic conductivities sufficient for use in batteries at elevated temperatures. According to previous studies the conduction of Li-ions within a block copolymer electrolyte occurs entirely within the centre of the microphase-separated PEO domains [1]. To potentially improve the conduction within the centre of the microphase-separated domains we added a low-viscosity, branched poly(ethylene oxide) (PEO^3) and Li-ions in the form of LiTFSI to a PS-PEO block copolymer. Impedance measurements of samples containing different combinations of PS-PEO, PEO^3 and LiTFSI are taken to find which is the most effective.

[1]Gomez, E. D.l Ashoutosh, P.; Feng, E. H.; Chen, V.; Stone, G. M.; Minor, A. M.; Kisielowski, C.; Downing, K. H.; Borodin, O,; Smith, G. D.; Balsara, N. P. Macromolecules 2009, 9, 1212.

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Olijve's Project Page - CISEI summer 2009

Intern: Luuk Olijve, Biomedical Engineering, Eindhoven University of Technology
Mentors: Ravinath Kausik, Sunyia Hussain,
Faculty supervisor: Songi Han
Department: Department of Chemistry and Biochemistry

The Effect of Cholesterol on Phospholipid Bilayers Studied by DNP Enhanced ^{1}H NMR

A fundamental study of biomembrane dynamics allows for a thorough understanding of the role of the cell membrane in regulating cellular processes. Cholesterol is a key component in the regulation of membrane fluidity and is essential for the formation of lipid rafts, which are centers for the assembly of signaling molecules in cell membranes. One way to study the effect of cholesterol on the dynamics of phospholipid bilayers is to study local water diffusion, since surface and internal water dynamics strongly regulate the macromolecular assembly and functioning of biological systems. Through the use of Dynamic Nuclear Polarization (DNP), the ^{1}H NMR signal of local water molecules is amplified via the interaction with nitroxide based spin labels localized on the surface and within phospholipid bilayers. By measuring the local hydration dynamics near the surface and across the bilayer, the effect of cholesterol on the dynamics of biomembranes can be determined. Electron Spin Resonance (ESR) is used as a complementary tool to provide insight into the effect of cholesterol on the dynamical properties of phospholipid bilayers, by studying the rotational dynamics of head and tail spin-labeled lipids within the bilayer. In a binary DOPC/cholesterol system, DNP and ESR studies confirmed that cholesterol significantly influences the interior dynamics of phospholipid bilayers. Large unilamellar vesicles containing 1:1 DOPC/DPPC and 30 mol% cholesterol are used as synthetic ternary biomembranes. DNP and ESR studies on this ternary biomembrane model are currently in process and will provide more insight into the effect of cholesterol on cell membranes.

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Rochford's Project Page - CISEI summer 2009

Intern: Brian Rochford,
Mathematics, University College Cork
Mentor: Robert Hoy
Faculty supervisor: Glenn Fredrickson
Department: Materials Research Laboratory

Simulations of Associating Polymers

Backbones of polymer chains are held together by permanent covalent bonds. In associating polymers there are a number of “sticky” monomers on the backbone. Those monomers form “sticky” bonds with each other that are comparatively weak and have a finite lifetime. When studying these associating polymers we must not only consider the complicated polymer physics, but also an added time and energy scale due to the sticky bond’s thermodynamics and chemical kinetics. Unfortunately, the dynamical and mechanical properties of associating polymers remains poorly understood. In order to overcome this, we use a model that exhibits: realistic dynamics, variable chemical kinetics and bonding reflective of typical experimental systems. The model chosen was based on the Kremer-Grest bead-spring model, which has been extensively validated and is known to capture the key physics of polymer melts. Implementation of this model yields large data sets that have previously been difficult to handle. We have developed a new approach to the data analysis which lets us calculate correlation functions to investigate certain aspects of the behaviour of these associating polymers. From these correlation functions we can further our understanding of the dynamical and mechanical properties of associating polymers.

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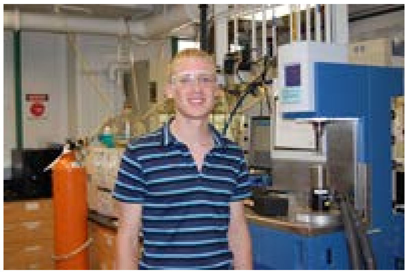

Intern: Stefan Schommer,
Materials Science, Saarland University, Germany
Mentor: Yanli Gong
Faculty supervisor: Gary Leal
Department: Chemical Engineering

Effects of Reactive Compatibilizer on Immiscible Polymer Blends

In general, compatibilization of polymer blends causes two major effects: First, it suppresses droplet coalescence, resulting in a smaller drop-size and a change in the related rheological properties, particularly in relaxation time. Second, the terminal complex viscosity is increased, which can be interpreted in terms of a partial surface immobilization. In this study, we analyze the rheological properties of concentrate blends of Polybutadiene (PBd) and Polydimethylsiloxane (PDMS) and the effects of adding a PBd-COO^{-} $^{+}H3N$-PDMS copolymer as a compatibilizer to these mixtures. Our samples were prepared by varying the volume fraction of PBd and PDMS in the polymer blend between 20:80 and 80:20. The experiments are then conducted on blends containing 0.1 or 1 wt. % of compatibilizer. All blends have a droplet matrix-structure with the major phase being the continuous phase. The rheological properties are analyzed over a series of frequency sweep experiments with decreasing pre-shear rates. In blends in which PBd forms the continuous phase, 1 wt. % of compatibilizer can suppress the coalescence of PDMS drops completely. This is not found in the 0.1 wt. % compatibilized case, or when PDMS is the continuous phase. Also, in blends with PBd as the continuous phase, the terminal complex viscosity is comparable to that of a suspension of rigid spheres, which suggests, that the interface has been immobilized almost completely.

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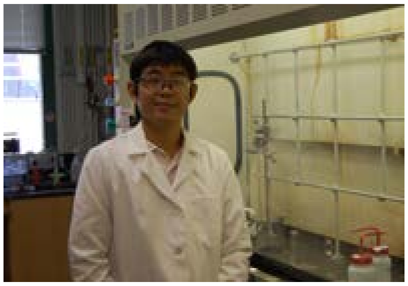

Intern: Min Tang,
Chemistry, Fudan University
Mentor: Joshua D. Furman
Faculty supervisor: Anthony K. Cheetham
Department: Materials Research Laboratory

Anthroquinone Luminescence in Inorganic-Organic Hybrid Framework Materials

Inorganic-organic hybrid framework materials, which are often described as extended crystals of metal atoms linked by organic ligands, have drawn much attention mostly in catalysis and gas storage. Recently, the phenomena under investigation in these structures have expanded to include magnetism, luminescence, conductivity and non-linear optical behavior. As phosphor materials for white-LED applications, photoluminescent hybrid frameworks can combine the stability of inorganic materials with the device compatibility and processing conditions of organic phosphors. Our approach is to insert intrinsically luminescent organic ligands between optically inert metal atoms to stabilize and tune the luminescence. We present a series of compounds containing the yellow luminescent 2,3-anthraquinone carboxylic acid with calcium, barium, manganese, nickel and zinc, prepared under hydrothermal conditions. The structures of these compounds have been characterized by single crystal X-ray diffraction and their photoluminescent emission and excitation spectra were collected at 77K. Thermal gravimetric analysis was used to measure their stability. We have seen trends such as cation emission shifting within this hybrid framework system that contribute to the understanding of photoluminescent hybrids as a new class of materials.

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