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Cooperative International Science and Engineering Internships

Cooperative International Science and Engineering Internships(CISEI)
Summer 2007 - Student Projects

Student/School	Mentor	Faculty Sponsor	Department	Student Project
Dan Feng Chemistry, Fudan University, Shanghai, China	Qihui Shi	Galen Stucky	Chemistry	Synthesis of Bifunctional or Multifunctional Core/Shell Nanoparticles
Christopher Fenwick MEng Engineering & Materials, University of Oxford, England	Mark White and Min-Ying Tsai	Jim Speck	Materials	Molecular Beam Epitaxy: Characterization and Growth of SnO_2
Martijn Gillissen Molecular Engineering, Technische Universiteit Eindhoven, Netherlands	Hunaid Nulwala	Craig Hawker	MRL	Reactivity Ratios of a Versatile New Monomer: Vinyl-triazoles
Sinead Griffin Theoretical Physics, Trinity College Dublin, Ireland	Kris Delaney	Nicola Spaldin	MRL	Thermoelectrics by Design
Sabine Haag Materials Science, Max Planck Institute for Metals Research, Stuttgart, Germany	Hongfei Lin	Eric McFarland	Chemical Engineering	Encapsulation of Nanoparticles in Mesoporous Silica
Eoin Hyde Mathematics and Applied Mathematics, University College Cork, Ireland	Anderson Janotti	Glenn H. Fredrickson	MRL	Phase Behavior of Block Copolymer/Star Polymer Mixtures
Cathal Leahy Theoretical Physics, Trinity College, Dublin, Ireland	Anderson Janotti	Chris van de Walle	MRL	Development of Visualization Tools for Computational Materials Science
Manuel Schnabel Materials Science, University of Oxford, England	Mark Dante	Thuc-Quyen Nguyen	Chemistry	Characterization of Diazapentacene Thin Films Containing Silver Nanoparticles Using Raman Spectroscopy and AFM

Benjamin Schwarz Materials Science, Max Planck Institute for Metals Research, Stuttgart, Germany	Wei Tang	Eric McFarland	Chemical Engineering	Electrocatalytic Activity of Au/Pt Nanoclusters for the Oxygen Reduction Reaction (ORR) in Fuel Cells

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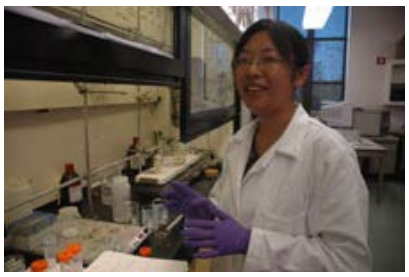
Feng's Project Page - CISEI summer 2007



Intern: Dan Feng, Chemistry, Fudan University, China
Mentor: Qihui Shi
Faculty supervisor: Galen Stucky
Department: Department of Chemistry

Synthesis of Bifunctional or Multifunctional Core/Shell Nanoparticles

Core/shell nanoparticles have attracted much attention in the field of material science because of their multi-functionality by controlling the composition, structure and interface of cores and shells. Much research has focused on the synthesis of such core/shell nanoparticles; however, most of the obtained products were monofunctional by taking advantage of either the core or the shell. Here we report the synthesis of a series of bifunctional or multifunctional core/shell nanoparticles comprising of superparamagnetic, optical, catalytic or stimuli-responsive properties in a single nanoparticle. The structure of a typical multifunctional core/shell nanoparticle is described as follows: a superparamagnetic (Fe_2O_3) core is prepared by the hydrothermal synthesis method, followed by coating with a soluable silica layer to stabilize the core. A porous ZrO_2 or TiO_2 layer which had potentials in the applications of bioseperation and enrichment of phosphopeptides was then coated on the surface of the silica shell, followed by a thermo sensitive polymer coating to control the availability of the overall nanoparticles. Lastly, catalytically active noble metal nanoparticles were embedded in the polymer shell by use of the stability effect of the polymer network to the metal nanoparticles. By combining the special features of the core and the shells, the overall nanoparticles are novel multifunctional ones, providing many kinds of applications in an entity. This work should have made a progress in the studies of functional nanoparticles.

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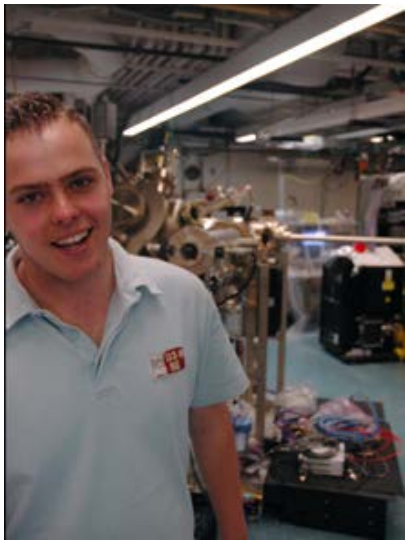
Fenwick's Project Page - CISEI summer 2007



Intern: Christopher Fenwick, MEng Engineering & Materials, University of Oxford, England
Mentor: Mark White
Faculty supervisor: Min-Ying Tsai and Jim Speck
Department: Materials Department

Molecular Beam Epitaxy: Characterization and Growth of SnO_2

Tin dioxide, SnO_2, is predominantly associated with gas-sensing applications via surface engineering and as thin film contacts, since it is a transparent-conducting oxide. A material's quality affects both its optical and electrical properties; therefore, improved growth parameters leading to high-quality crystalline structures will better utilize the high mobility and wide band gap (Eg ~3.6eV) inherent to SnO_2.

To date, SnO_2 films have been created via methods which produce polycrystalline or otherwise structurally-limited, impure material. Molecular Beam Epitaxy (MBE) is an ultra-high vacuum technique used for high-quality thin film growth of compound semiconductors with monolayer control. Using plasma-assisted MBE, research focused on structural coherency and purity will both lead to the advancement of electrical and optical properties and their understanding.

Different substrates are used for heteroepitaxy growth including Al_2O_3(1-1 02) (r-sapphire), TiO_2(110), and TiO_2(001). A range of characterization equipment determined the material properties for comparative analysis. X-Ray Diffraction, Atomic Force Microscopy, cross-sectional Scanning Electron Microscopy, and Hall Effect measurements were used to determine the film purity / crystallographic orientation, surface morphology / roughness, thickness, carrier mobility and concentration.

Optical measurements were conducted in the $300 < \lambda < 1000$nm wavelength range, using a variable angle spectroscopic ellipsometer. Assuming a homogeneous SnO_2 thin film, the sample was modeled using a parametric semiconductor that enables the refractive index and extinction coefficient to be calculated from the experimental data.

By understanding the relationships between film growth and properties, fundamental advancements may occur; work will progress towards creating a new class of semiconductors using oxides.

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Gillissen's Project Page - CISEI summer 2007

Intern: Martijn Gillissen, Molecular Engineering,
Technische Universiteit Eindhoven, Netherlands
Mentor: Hunaid Nulwala
Faculty supervisor: Craig Hawker
Department: MRL

Reactivity Ratios of a Versatile New Monomer: Vinyl-triazoles

Vinyl-triazoles are unique new polymerizable monomers. They allow facile incorporation of functionalities, possess an aromatic core and are capable of hydrogen bonding. The triazole core is highly modular and by utilizing different synthetic approaches 1,4 and 1,5 triazoles can be synthesized.

In this study the reactivity ratios of two 1,4 vinyl-triazoles were determined to be $r_{styrene}$ = 1.49 and $r_{1,4\text{-}BnTz}$ = 0.46 for 1,4 vinylbenzyl-triazole and $r_{styrene}$ = 1.83 and $r_{1,4\text{-}OctTz}$ = 0.45 for 1,4 vinyloctyl-triazole, which are both indicative for random co-polymerization. To determine these reactivity ratios, copolymerization reactions of the vinyl-triazole monomers with styrene at feed ratios between 10% to 90% styrene were carried out, keeping conversions low to avoid compositional drift. The reactivity ratios were then obtained by nonlinear least squares fitting the composition of the obtained polymers, determined by ^{1}H-NMR, to the Mayo-Lewis equation. In addition 95% joint confidence intervals for the reactivity ratios were determined.

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Griffin's Project Page - CISEI summer 2007

Intern: Sinead Griffin, Theoretical Physics, Trinity College Dublin, Ireland
Mentor: Kris Delaney
Faculty supervisor: Nicola Spaldin
Department: MRL

Thermoelectrics by Design

Vinyl-triazoles are unique new polymerizable monomers. They allow facile incorporation of functionalities, possess an aromatic core and are capable of hydrogen bonding. The triazole core is highly modular and by utilizing different synthetic approaches 1,4 and 1,5 triazoles can be synthesized.

A thermoelectric device is one that enables the conversion of a temperature difference into an electrical current. Good electrical and poor thermal conductivity are necessary prerequisites for an efficient thermoelectric device. There is a great demand for novel thermoelectric materials, and theoretical understanding of the origin of their properties. One proposed new compound is lanthanum-doped strontium titanate. Here, we investigate the addition of lanthanum doping in oxygen-deficient strontium titanate to explore the enhancement of thermoelectric-relevant properties. Pure strontium titanate forms a perovskite structure, a structure that is also important for ferroelectric materials and high-T_c superconductors. The atomic and electronic structure of oxygen vacancies, the primary mechanism for transforming the insulating strontium titanate into a good electrical conductor, has been studied previously using ab initio simulation techniques. We first investigated pure strontium titanate using Density Functional Theory applied to a periodic simulation cell. The lattice constant, band structure and density of states of the ideal perovskite structure, with the Pm3m space group, were confirmed. At low temperatures, the lattice perturbs, and a relaxation was carried out on this canted lattice. This phase was used to investigate properties of an oxygen-deficient crystal. Finally, lanthanum doping was introduced and the effect on the electronic structure studied.

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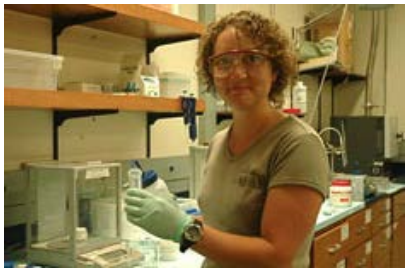
Haag's Project Page - CISEI summer 2007



Intern: Sabine Haag, Max Planck Institute for Metals Research, Stuttgart, Germany
Mentor: Hongfei Lin
Faculty supervisor: Eric McFarland
Department: Chemical Engineering

Encapsulation of Nanoparticles in Mesoporous Silica

Vinyl-triazoles are unique new polymerizable monomers. They allow facile incorporation of functionalities, possess an aromatic core and are capable of hydrogen bonding. The triazole core is highly modular and by utilizing different synthetic approaches 1,4 and 1,5 triazoles can be synthesized.

The surface area of nanoparticles is extremely high, which could be used advantageously in catalysis and provide a maximum capacity for solid reactants. Unfortunately, deactivation by sintering at elevated temperature limits their use. To stabilize nanoparticle solid reactants against sintering while maintaining their capacity and activity, mesoporous coatings with an adjustable pore size can be designed to allow reactant gases and liquids in, but prevent the active solid from leaving.

To synthesize the mesoporous silica, TEOS (Tetraethoxysilane) and C_{18}-TMS (Octadecylmethoxysilane) were used as precursors in a modified Stöber process. C_{18}-TMS forms micelles that are encased during the co-condensation and therefore increase the porosity after calcination.

Silica, nickel oxide, copper oxide, zinc oxide and calciumcarbonate were used as core materials. TEM, SAXS, BET and capacity measurements were performed to characterize the products. The final structure is highly dependent upon pH, the water to ethanol ratio, and the relative surface energies of the core and shell materials.

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Hyde's Project Page - CISEI summer 2007

Intern: Eoin Hyde, Mathematics and Applied Mathematics, University College Cork, Ireland
Mentor: Folusho Oyerokun and Dominik Düchs,
Faculty supervisor: Glenn H. Fredrickson
Department: MRL

Phase Behavior of Block Copolymer/Star Polymer Mixtures

Diblock copolymer melts have long been known to exhibit microphase separation at temperatures below a threshold order-disorder temperature and to thus self-assemble into a host of morphologies – lamellar, cylindrical, gyroid, spherical – depending on the volume fractions of the constituent blocks. The addition of gold nanoparticles with short chains of either or both of the diblock monomeric species grafted onto their surfaces has recently been demonstrated through both experiments and hybrid particle/field simulations to significantly alter the phase behavior of the combined system in relation to that of the pure diblock. In particular, neutrally coated particles, i.e. those with equal numbers of each diblock species grafted onto their surfaces, cause the system to form bicontinuous microemulsions, a technologically relevant morphology not observed in the pure diblock. The aim of the present project is to mimic the effect exerted by such neutrally coated particles by replacing them with symmetric star polymers. We study this system through mean-field, or thermally equilibrated, calculations within the framework of the well-known Self-Consistent Field Theory for polymer melts. After a preliminary investigation of the special case of a long and short diblock, we were indeed able to observe microemulsions in the AB + A4B4 system. Further study shall be directed at more thoroughly understanding the phase behavior of this class of systems by varying the number of arms in the stars as well as volume fractions, interaction parameters, and l ength ratios.

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Leahy's Project Page - CISEI summer 2007

Intern: Cathal Leahy, Theoretical Physics, Trinity College, Dublin, Ireland
Mentor: Anderson Janotti
Faculty supervisor: Chris van de Walle
Department: MRL

Development of Visualization Tools for Computational Materials Science

Visualization tools are important in understanding and analyzing data produced by first-principles calculations. Density functional theory uses the electronic charge density as its basic parameter as opposed to the many body wavefunction. This reduces a 3N-dimensional problem, where N is the number of electrons, to a set of single particle equations in 3 dimensions. The charge density contains information on chemical bonding and, thus, on the electronic and structural properties of solids and molecules.

This project seeks to improve a user-friendly visualization code based on **OpenDX** used in the visualization of charge densities. It involves the manipulation of a C code, which converts the output data from first-principles calculations, as well as programming in the OpenDX environment. The pre-existing codes only allowed for visualization of one supercell. In this project the C code was modified to replicate this supercell in the 3D space in order to resolve features that are near the supercell boundaries. It is now possible to replicate the atom coordinates, charge densities and the connectivity between atoms (bonds) in all directions. The user can specify the multiplicity and the directions in which the supercell is to be replicated. New modules within OpenDX were developed to provide an enhanced image of contour lines and isosurfaces of charge densities. Within OpenDX a main control panel was set up so that all the imaging tools can be easily accessed and altered. A user guide has also been prepared in order to facilitate the use of the visualization tools by other research groups.

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Schnabel's Project Page - CISEI summer 2007

Intern: Manuel Schnabel, Materials Science, University of Oxford, England
Mentor: Mark Dante
Faculty supervisor: Thuc-Quyen Nguyen
Department: Chemistry

Characterization of Diazapentacene Thin Films Containing Silver Nanoparticles Using Raman Spectroscopy and AFM

Organic semiconductors have a vast range of potential applications in flexible displays, photodiodes, solar cells and sensors. 6,13-diazapentacene is a novel organic semiconducting material having cofacial packing and thus presumably high charge mobility. When gold or silver electrodes are deposited on top of the diazapentacene film, AFM images show the electrode metals diffuse onto the film to form nanoparticles. Images taken a week after deposition do not show more nanoparticles, but the ones present are larger, implying that coarsening then outstrips diffusion. Raman spectroscopy was used to determine whether the silver nanoparticles enhance the Raman signal of the diazapentacene, as this would permit this hybrid material to be used in sensors. However we did not observe significant Raman enhancement, neither immediately after deposition nor over time. This may be due to the small number of nanoparticles that diffused, preventing the formation of 'hot spots', i.e. clusters of nanoparticles which lead to very strong Raman enhancement. Annealing the sample at successively higher temperatures actually decreases the Raman intensity, again suggesting that coarsening occurs faster than diffusion. Addition of 1nM silver nanoparticle solution lead to some enhancement, indicating that the absence of Raman enhancement during diffusion can be attributed solely to diffusion of silver as nanoparticles that are not Raman enhancers. This precludes the use of a diazapentacene-silver nanoparticle hybrid for sensors unless a way is found to promote nanoparticle clustering.

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Schwarz's Project Page - CISEI summer 2007

Intern: Benjamin Schwarz, Materials, Max Planck Institute for Metals Research, Stuttgart, Germany
Mentor: Wei Tang
Faculty supervisor: Eric McFarland
Department: Chemical Engineering

Electrocatalytic Activity of Au/Pt Nanoclusters for the Oxygen Reduction Reaction (ORR) in Fuel Cells

Fuel cells are one of the oldest electrical energy conversion technologies, invented in the middle of the 19th century. There are numerous applications for fuel cells, for example portable power devices (Cell Phones, Notebooks), vehicle propulsion or power plants. Furthermore, fuel cells can contribute to the reduction of emissions thanks to their high efficiency. To achieve high efficiencies it is necessary to use a catalyst for the reduction of oxygen ($O_2 + 4\,H^+ + 4\,e^- \rightarrow 2\,H_2O$). The most commonly used material is platinum. However platinum is rare and very expensive. The aim of this project is to characterize Au/Pt alloy electroreduction catalysts that minimize the platinum content by using cheaper and more abundant gold.

In order to determine the activity of different Au / Pt ratios, a rotating disk electrode (RDE) was used at variable rotation speeds to distinguish mass transfer from chemical reaction kinetics. The working electrode is a carbon disk whereon the Au / Pt nanoclusters are deposited by electrodeposition. It was able to show, that in an acidic environment, Au doped Pt improves the oxygen reduction and in an alkaline electrolyte, both Au and Pt, are active for the oxygen reduction.

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