

Poster Presentation
May 2, 2014
12:30-2:00 p.m.
Hesburgh Library Concourse

The Maximum Loading Capacity of Platinum on Cerium Oxide Catalysts

Joy Tao
College of Science
Science-Business

Advisor: Franklin Tao, University of Notre Dame, College of Science, Department of Chemistry and Biochemistry

The water-gas shift (WGS) reaction is essential in the production of hydrogen for fuel cell power generation and carbon monoxide conversion. Carbon monoxide in particular needs to be completely converted because it poisons platinum electrodes, obstructing fuel cell performance, and it is a noxious pollutant. Cerium oxide, when loaded with noble metals such as platinum, is a very effective WGS catalyst at lower temperatures. Transition metals enhance the reducibility of ceria, and single dispersed metals on ceria support are more reactive than clusters of metals because of the enhanced oxygen migration on the CeO_2 surface. In the case of CeO_2 impregnated with platinum, CO molecules absorbed on the platinum is oxidized to CO_2 by the migration of an oxygen to the metal-cerium interface, and water is reduced and dissociates on the oxygen vacancy sites of ceria to H_2 . Large clusters of Pt particles will have insignificant interactions with ceria, but the total number of highly dispersed platinum particles will increase with loading. In this experiment, the maximum loading amount of platinum on CeO_2 while still being singly dispersed after reaction was explored. CeO_2 nanorods were prepared via hydrothermal methods at 100°C by mixing cerium nitrate with sodium hydroxide. Platinum supported catalysts at 0.05%, 0.1%, and 0.5% were prepared using deposition-precipitation method. Gas chromatography is used to analyze the efficiency of the Pt/ CeO_2 at different loading percentages for catalyzing the WGS reaction and for calculating the turnover frequency (TOF) of the catalyst. The results of this experiment can be applied to many different nanocatalysts and reactions related to energy systems.

Poster Presentation
May 2, 2014
12:30-2:00 p.m.
Hesburgh Library Concourse

Implications of Multicomponent Diffusion Effects for Forward Osmosis Water Treatment Systems

Alex Oloriz
College of Engineering
Chemical Engineering

Advisor: William A. Phillip, University of Notre Dame, Department of Chemical and Biomolecular Engineering

Forward osmosis (FO) is an emerging method of water treatment that is finding various applications (*e.g.*, desalination of high-salinity brines, wastewater reclamation, treatment of produced water). Several recent experimental studies have indicated that multicomponent diffusion effects can influence the performance of FO systems. In a system where multicomponent effects are present, the concentration of one solute can either enhance or retard the permeation of another solute. Enhanced solute permeation in FO can diminish the ability of a system to reject harmful contaminants. Therefore, understanding and quantifying the influence of these multicomponent effects on membrane performance at a systems level is necessary to aid in the design and implementation of novel FO systems.

This study seeks to quantify the effects of multicomponent diffusion on the performance of novel water treatment systems. Specifically, physiochemical models, which can be solved analytically in relevant physical limits, are developed. Analytical models for both co-current and counter-current membrane contactors are derived and solved in the limit that the water flux is negligible. The resulting models yield physical insight into the behavior of FO systems where a variety of multicomponent diffusion effects are present, and establish a foundation for further numerical modeling. Initial numerical studies for co-current operation, which account for the effects of a water flux, were conducted. The results from the numerical model match the results from the analytical solution well in the limit that the water flux approaches zero. Importantly, both models predict that multicomponent diffusion will have a greater effect on the permeation of dilute species than on the permeation of more concentrated solutes. These models, which are useful tools for understanding the influence of multicomponent diffusion effects on FO systems, will ultimately allow for the prediction of systems level performance based on lab scale membrane characterization.

Poster Presentation
May 2, 2014
3:15-4:45 p.m.
Hesburgh Library Concourse

Hole Mobility in Solid State Cadmium Chalcogenide QDSCs

Timothy Siegler
College of Engineering
Chemical Engineering

Advisor: Prashant Kamat, University of Notre Dame, Colleges of Science and Engineering, Departments of Chemistry and Biochemistry, Chemical and Biomolecular Engineering, and Radiation Laboratory

Quantum Dot Solar Cells (QDSCs) are promising candidates for production of high efficiency photovoltaic devices, due to their high molar extinction coefficients, their ability to be processed in solution, and their tunable band gap. A primary goal in this field is to make solid state QDSCs, due to their relative stability and flexibility compared to liquid junction devices. However, to date, there have been very few studies on solid state cells employing the otherwise popular CdX absorber, where X= S, Se, or S(x)Se(1-x). Common state of the art technologies suffer from recombination at the hole transporting material (HTM), and therefore produce inefficient solar cell devices.¹

In this project, hole transport dynamics are directly measured using transient absorbance spectroscopy for CdS, CdSe, and CdS(x)Se(1-x) via measurement of the absorbance of chalcogenide radicals on the surface of the active electrode. Then, ss-QDSCs are constructed utilizing a novel HTM, copper zinc tin sulfide (CZTS), and cell performance measured under 1 sun illumination. Since CZTS is a visible light absorber, it should show increased hole transfer and recombination lifetimes under illumination. Therefore, hole and electron transfer rates as well as recombination lifetimes of this HTM on CdX are measured using transient absorption spectroscopy and open circuit voltage decay, and show how CZTS acts as a HTM in these devices.

1. Roelofs, K.; Brennan, T.; Dominguez, J.; Bailie, C.; Margulis, G.; Hoke, E.; McGehee, M.; Bent, S. Effect of Al₂O₃ Recombination Barrier Layers Deposited by Atomic Layer Deposition in Solid-State CdS Quantum Dot-Sensitized Solar Cells. *Journal of Physical Chemistry C* 2013, 117 (11), 5584-5592.

Poster Presentation
May 2, 2014
3:15-4:45 p.m.
Hesburgh Library Concourse

Synthesis and Characterization of UV Curable Aromatic Polyimide Membranes for High Performance Gas Separation Applications

Christopher Walker
College of Engineering
Chemical Engineering

Advisor: Ruilan Guo, University of Notre Dame, College of Engineering, Department of Chemical and Biomolecular Engineering

Membrane separations offer a low-cost, environmentally-friendly alternative to energy-intensive staged equilibrium operations, the current standard. Polymeric membranes that exhibit an optimal balance of gas selectivity and permeability have great potential for efficiently separating gas mixtures such as carbon dioxide and methane or oxygen and nitrogen, both highly prevalent industrially. However, drawbacks that have prevented the widespread use of polymer membranes for industrial gas separations are that they have relatively low chemical resistance, most notably resistance to carbon dioxide-induced plasticization, and sometimes insufficient mechanical and thermoxidative stability.

One possible way of overcoming these limitations is to use a cross-linked polymer. Cross-linked polymers, in which chains are interconnected by covalent bonds, are more robust and have smaller microcavities, potentially offering high chemical resistance, mechanical strength, and selectivity, but at the expense of gas permeability. In this project, a UV curable copolyimide scheme comprised of three monomers is proposed: an aromatic diamine with bulky methyl side groups, an aromatic dianhydride with bulky trifluoromethyl groups, and a second aromatic dianhydride which contains a UV-sensitive benzophenone moiety. The bulky side groups promote high gas permeability; the benzophenone group allows for potential cross-linking; and the aromatic rigid backbone contributes to relatively high mechanical strength. A series of aromatic polyimides with varying composition was synthesized in the laboratory by solution imidization, and membrane films were cast on glass plates. By varying the monomer composition, the potential cross-link density varies accordingly. These copolyimides were comprehensively characterized in terms of their chemical structures (via ¹H NMR and FTIR) and thermal properties (by DSC and TGA). Upon film forming, UV crosslinking will be applied to these polyimide films at systematically varied levels of intensity and irradiation time to afford crosslinked membranes with controlled crosslink density, which will be evaluated via gel fraction measurements. Pure gas permeation tests will then be performed on both linear controls and the cured membranes to establish the fundamental structure-property relationship for these UV crosslinked polyimide membranes to maximize both the transport properties and chemical resistance of the membranes.

Oral Presentation

August 2, 2013 (Summer Undergraduate Research Symposium)

Exploration of Design of Experiments for Understanding Competitive Balance between Embodied Energy and Operational Energy in Buildings

Clarissa Rogg
College of Engineering
Civil Engineering

Advisors: David Go, University of Notre Dame, College of Engineering, Department of Aerospace and Mechanical Engineering, and Aimee Buccellato, University of Notre Dame, School of Architecture, Department of Architecture

Buildings accounted for almost 40% of the total energy consumed by the United States in 2012. Reducing the energy consumption of buildings is recognized as a national priority, and there is now an increased need to optimize the energy performance of a building during the design process. The total energy used in buildings is attributed to either the operational energy, or energy used to operate the building during its lifetime, or embodied energy: the energy used to create the materials in the building. Optimizing the energy efficiency of buildings is inherently complicated since there are numerous variables to consider. Design of Experiments (DoE) is an analysis method that reduces the necessary number of runs of an experiment in order to identify the main effects of each variable on a complex system. When combined with the Response Surface method, a single equation predicting the response to multiple variables can be established and subsequently optimized. For this work, the DoE approach is used to understand how different variables for the window configuration of a building model affect both the operational and embodied energy performance of the building. The building models are created in SketchUp and simulated in the energy analysis program, EnergyPlus. DoE is used to identify which variables impact operational energy, embodied energy, and total energy. For this model system, the variables that have the greatest impact on operational energy do not always have the greatest impact on embodied energy, highlighting the inherent competitive balance between design choices that impact energy performance.

Poster Presentation

August 2, 2013 (Summer Undergraduate Research Symposium)

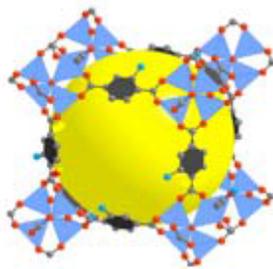
Synthesis of IRMOF-3 and Conversion of Dihydroxyacetone to Ethyl Lactate

Hamim Nigena

Morehouse College, Applied Physics and Electrical Engineering

Advisor: Jason Hicks, University of Notre Dame, College of Engineering, Department of Chemical and Biomolecular Engineering

The goal of my research project was two-fold: 1) synthesizing a post-synthetically modified Sn-containing metal organic framework (MOF), Sn-IRMOF-3, and 2) the catalytic conversion of dihydroxyacetone (DHA) to ethyl lactate (EL) with the carbonized MOF (Sn/NC). The synthesis of the MOF, which contained an amine functionality, involved a solvothermal approach, using N,N-dimethylformamide (DMF), $Zn(NO_3)_2 \cdot xH_2O$, and 2-aminoterephthalic acid as a reaction solvent, a precursor for metal oxide cluster, and an organic linker, respectively. The resulting MOF (denoted as IRMOF-3) possessed microporosity with high surface area (BET surface area of 980 m²/g, and a Langmuir surface area of 1370 m²/g) as well as a ~ 100 nm-sized cubic structure (obtained by SEM). The IRMOF-3 was modified by metallation with a Sn-precursor. Subsequently, the Sn-IRMOF-3 was carburized to generate a Sn/NC material. The catalytic conversion of DHA to EL was then studied under relatively mild conditions using the Sn/NC material as a catalyst. The average particle size of Sn on the nanoporous carbon support was ~ 100 nm via TEM, and the Sn was considered highly dispersed on the nanoporous carbon based on the lack of a tin oxide diffraction pattern in X-ray diffraction experiments. Lastly, the Sn/NC was exhibited a high activity toward the catalytic conversion of DHA, and this catalyst can be a promising material for the production of ethyl lactate, a raw material for the synthesis of a biodegradable polymer. Future studies will involve the catalyst stability under reaction conditions, as Sn leaching was observed in the reaction media.



Poster Presentation

August 2, 2013 (Summer Undergraduate Research Symposium)

Thiolated gold and silver nanoclusters absorption of visible light

Julian Pilate-Hutcherson
Morehouse College, Applied Physics

Advisor: Prashant Kamat, University of Notre Dame, Colleges of Science and Engineering, Departments of Chemistry and Biochemistry, Chemical and Biomolecular Engineering, and Radiation Laboratory

Abstract:

The absorption of thiolated gold and silver nanoclusters can be tuned in the visible (350 and 700 nm) region. Unlike their counterpart of larger nanoparticles, these few atom nanoclusters do not exhibit plasmon absorption, but exhibit molecular-like properties. Upon visible excitation, these nanoclusters are capable of injecting electrons into TiO₂. There were several methods tested for the synthesis of these thiolated gold clusters, in every case Au³⁺ was reduced to Au⁰ in the presence of glutathione as a stabilizing agent. In one method Au³⁺ was reduced by refluxing with glutathione as the reducing agent. In other experiments Au³⁺ was reduced, at room temperature, by NaBH₄ in the presence of glutathione. In yet another set of experiments silver nanoparticles were used in galvanic exchange to reduce Au³⁺, while they themselves become oxidized. Silver nanoclusters were also synthesized by reduction with the addition of NaBH₄ again in the presence of glutathione as a stabilizing agent. All the synthesized gold and silver nanoclusters were able to absorb an appreciable amount of visible light up to 650 nm. These gold or silver clusters that absorb visible light may provide increased efficiency of TiO₂ solar cells by absorbing more sunlight.

Final Report:

The project I have been working on this summer is synthesizing stable gold and silver clusters that absorb visible light (350 and 700 nm). This project is important because these clusters are able to provide increased efficiency by absorbing more sunlight when absorbed onto TiO₂ film. In addition to this, this class of sensitizers will lead to other studies of metal clusters that may be able to absorb an appreciable amount of light. These gold and silver clusters were made in various ways. Each type of clusters synthesis involved glutathione as a stabilizing agent. Glutathione was used for the Ag or Au clusters in making these clusters because of its ability to bind to gold and silver and provide water solubility of these clusters.

The thiolated Au clusters were made by three methods. Gold clusters were made by heating Au³⁺ ions in the presence of glutathione to 70⁰ Celsius for 24 hours.¹ These clusters were seen to have an increased light absorbance up to 450 nm. We also made these clusters by refluxing Au³⁺ ions with glutathione for 3 hours. An absorbance spectrum was taken every 30 minutes for three hours, and it was observed that the refluxed gold clusters after 3 hours had similar properties as the clusters that were made when heated at 70⁰ for 24 hours. These clusters absorb a significant

amount of light between 350 and 500 nm in the visible region and have been previously shown to give >2 % efficient solar cells. The absorbance spectrum of these clusters can be seen in Figure 1.

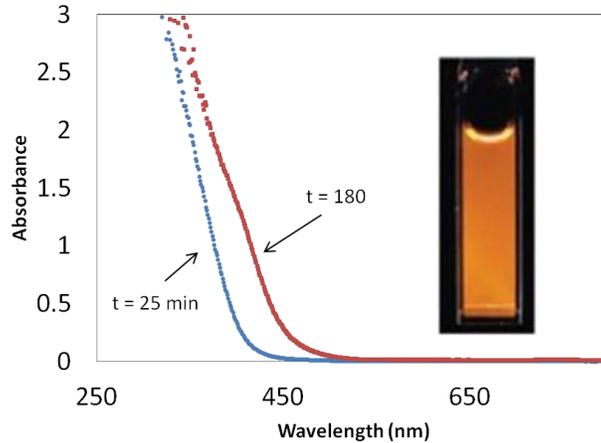


Figure 1 illustrates the increase of absorbance between gold clusters refluxed for 30 minutes and 180 minutes. At 180 minutes, the gold clusters had an absorbance up to 400 nm.

In order for the gold clusters to be more photoactive, it is necessary to control the optical properties of the clusters to ensure that they absorb appreciable visible light. In the second method, the glutathione reduced Au^+ ions were reduced again by $NaBH_4$ (0.1, 0.5, 1, 5, and 10 sodium borohydride equivalent amounts were added to Au^+ ions). It was seen that when 0.1 and 0.5 equivalences were added to the nanoparticles, the clusters' had low absorbance levels, however, increased dramatically as 1, 5, and 10 equivalences were added. 0.1, 0.5, and 1 equivalences heavily precipitated to the bottom of the samples, while the 5 and 10 equivalent samples remained a dark purple color. The gold with the 10 equivalent samples of $NaBH_4$ had absorption bands up to 500 nm, which may provide increased efficiency of TiO_2 solar cells by absorbing more sunlight. An absorbance spectrum of the glutathione and $NaBH_4$ reduced clusters can be seen in Figure 2, to illustrate the increase in absorbance achieved by sodium borohydride reduction.

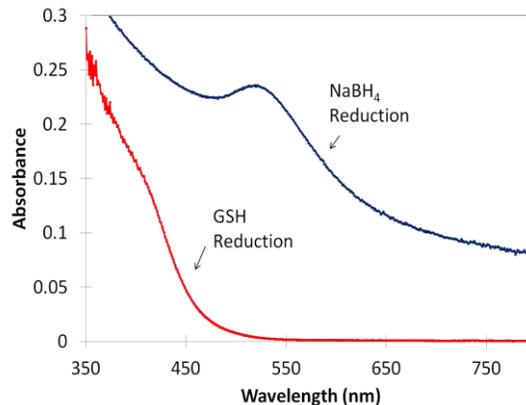


Figure 2 compares the absorption bands between gold nanoclusters reduced by only glutathione and clusters reduced by glutathione and the addition of NaBH₄. The nanoclusters reduced by NaBH₄ absorbed light up to 500 nm.

The third method in which gold clusters were synthesized was by having silver nanoparticles reduced by sodium borohydride and stabilized by trisodium citrate undergo galvanic exchange to reduce Au³⁺, while they themselves become oxidized. The silver particles without adding the Au³⁺ had a peak absorbance at 400 nm, however with an introduction of HAuCl₄, the absorbance was red shifted. There was an increase in absorbance of visible light at 470 nm with the introduction of 0.05 mM, 0.1 mM, and 0.2 mM of HAuCl₄ and these clusters also remained stable. These clusters absorb an appreciable amount of visible light between 300 and 600 nm. However, with the introduction of 0.5 mM and 1 mM of HAuCl₄, the absor

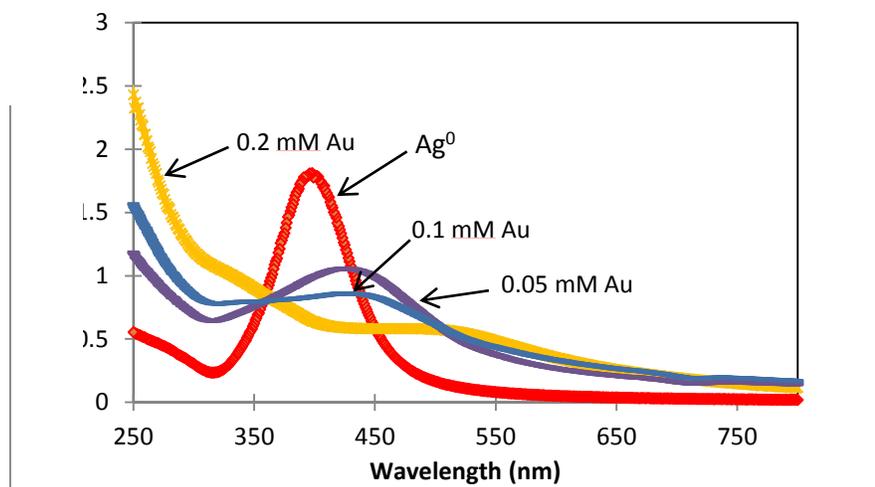


Figure 3 illustrates the absorbance spectra of the silver nanoclusters compared to the gold clusters formed by the addition of Au³⁺ ions. The gold clusters formed when 0.1 mM of Au³⁺ ions were added had an increase of absorbance up to 470 nm.

In addition to the gold nanoclusters, silver nanoclusters were also synthesized. Silver clusters also have a high potential for creating highly efficient solar cells. These silver clusters were made by reducing Ag⁺ to Ag⁰ by the introduction of NaBH₄ as the reducing agent, in the presence of glutathione. Once the silver ions were reduced twice, the clusters were able to absorb light up to 640 nm.² An experiment was also done to see if the thiolated silver nanoclusters can be made more emissive. According to an article, silver nanoclusters can be made more emissive by being passed through a desalting column which would remove excess ligands and salts that inhibit emission. After obtaining the desalting column and following the article procedure, the clusters were not able to emit light very strongly. After comparing the absorbances before and after being put through the desalting column, it was deduced that the desalting column did not have a significant effect on the silver clusters. The silver nanoclusters made in both experiments were not able to remain stable after 24 hours unless kept in an inert atmosphere. Illustrations and absorptions spectrums of the silver nanocluster experiments can be seen in Figure 4 and 5.

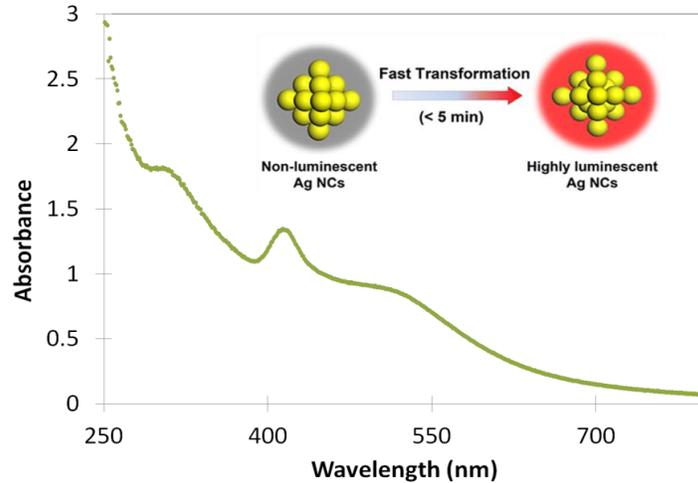


Figure 4 shows the absorbance spectrum of the silver nanoclusters formed when silver ions were reduced by NaBH_4 and a diagram illustrating the transformation of silver nanoclusters from non-luminescent to highly luminescent by being passed through a desalting column. The silver nanoclusters had an absorbance up to 600 nm.

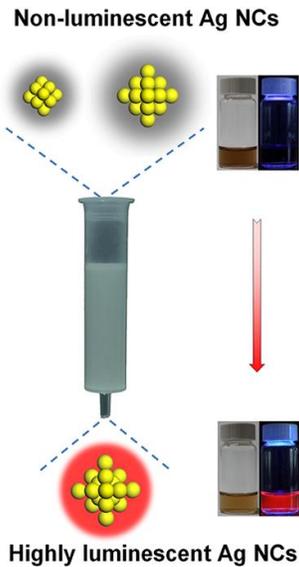


Figure 5 illustrates silver nanoclusters being passed through a desalting column and being transformed from non-luminescent to highly luminescent.

After being made, the nanoclusters were then absorbed onto TiO_2 film and tested on liquid junction solar cells with Co(II)/Co(III) electrolyte. Although the cells of both gold and silver nanoclusters were not able to generate much current, they were functional. The Au clusters were able to generate an open circuit voltage of about 0.8 V, while the Ag clusters generated about 0.45 V. The IV curve of these cells can be seen in Figure 6.

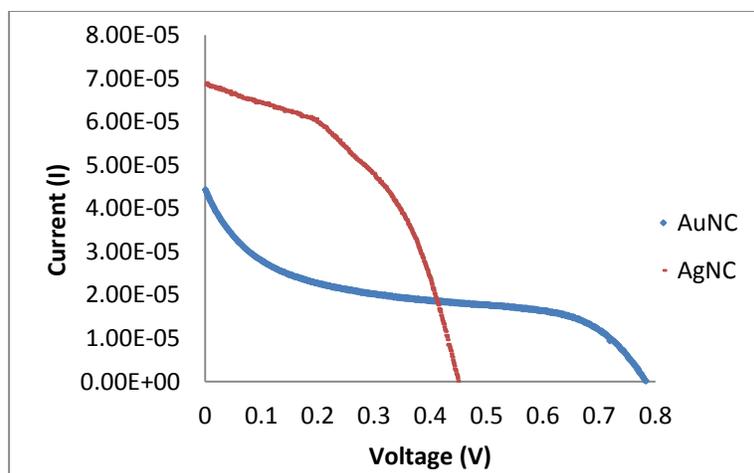


Figure 6 illustrates the IV curve of the most efficient gold and silver nanocluster sensitized solar cells.

Future works in this project include synthesizing more stable silver nanoclusters and generating a higher current out of both gold and silver nanocluster sensitized solar cells. These experiments this summer have shown that the gold or silver clusters that absorb visible light have potential for increasing the absorption of TiO₂ film in more highly efficient solar cells. These solar cells will then be able to convert more light energy from the sun into electricity.

References:

- (1) Zhentao Luo, Xun Yuan, Yue Yu, Qingbo Zhang, David Tai Leong, Jim Yang Lee, and Jianping Xie, From Aggregation-Induced Emission of Au(I)-Thiolate Complexes to Ultrabright Au(0)@Au(I)-Thiolate Core-Shell Nanoclusters. *J. Am. Chem. Soc.* **2012**, 134, 16662–16670
- (2) Xun Yuan, Qiaofeng Yao, Yong Yu, Zhentao Luo, Xinyue Dou, and Jianping Xie, Traveling through the Desalting Column Spontaneously Transforms Thiolated Ag Nanoclusters from Nonluminescent to Highly Luminescent. *J. Phys. Chem. Lett.* **2013**, 4, 1811–1815

Poster Presentation
February 2014 (Undergraduate Energy Research Expo)

GreenScale Research Project

Kendra Harding
College of Engineering
Civil and Environmental Engineering and Earth Sciences

Advisor: Aimee Buccellato, University of Notre Dame, School of Architecture, Department of Architecture

Project Overview

Current discussion of “green” building practices often assumes a correlation between sustainability and advanced building technologies. Much research is focused on the capabilities of modern technology to generate “sustainable” design solutions. The main goal of the GreenScale Research Project is to measure the true impacts associated with different building materials and methods of assembly.

The GreenScale Research Project has done a quantitative analysis of construction methods, materials, and principles of design through a series of original case studies focused on measuring, evaluating, and comparing purportedly “green” materials and methods of assembly alongside their traditional predecessors.

The team is currently developing a digital tool that will provide a comprehensive method for modeling the true costs of materials, methods, and designs in real time. The tool will give not only offer a way to select the “greenest” design on a case by case basis but will be a way to train students and designers in truly sustainable design choices.

Research Performed

Throughout the course of the school year I was involved in a number of subprojects. The first task I was involved with was research into the current availability of material information databases for building materials. This involved literature reviews of a number of online and published sources. In conjunction with this effort I developed of a pseudo-database to be used in testing the new programs being designed for the GreenScale project’s digital tool. This involved assembling data from a variety of sources.

The second major subproject I was involved with was the development of Life Cycle Assessment capabilities. Life Cycle Assessment is a methodology for evaluating comprehensive environmental impacts of individual products. In an effort to coordinate the GreenScale Tool with accepted methodology I did research into the current state of Life Cycle Analysis practice. From this I was able to help establish a methodology that could be used by the digital tool. As part of a smaller study I worked with local company Kuert Concrete to develop a case study of a Life Cycle Assessment.

Poster Presentation

November 2013 (IMECE Conference, San Diego, California)

Energy Harvesting for Thermal Energy Mechanisms and Applications

Patrick McFarlane
College of Engineering
Aerospace and Mechanical Engineering

Advisor: Fabio Semperlotti, University of Notre Dame, College of Engineering, Department of Aerospace and Mechanical Engineering

This work develops a mathematical model for an alpha Stirling refrigerator with air as the working fluid which will be useful in optimizing the mechanical design of these machines. Two pistons cyclically compress and expand air while moving sinusoidally in separate chambers connected by a regenerator, thus creating a temperature difference across the system. A complete non-linear mathematical model of the machine including air thermodynamics, heat transfer from the walls as well as heat transfer and fluid resistance in the regenerator is developed. Non-dimensional groups are derived, and the mathematical model is numerically solved. The heat transfer and work are found for both chambers, and the coefficient of performance of each chamber is calculated. Important design parameters are varied and their effect on refrigerator performance determined. This sensitivity analysis, which shows what the significant parameters are, is a useful tool for the design of practical Stirling refrigeration systems.

Simulation of Core-Shell Upconverting Nanostructures in Semiconductor Materials

Alexander Wentzel
College of Engineering
Electrical Engineering

Advisor: Mark Wistey, University of Notre Dame, College of Engineering, Department of Electrical Engineering

The purpose of Core-Shell Upconverting Nanostructures (CSUNs) is to create potential wells in semiconductor materials to trap electrons or holes, and create longer lifetimes of generated electron-hole pairs. This would be able to increase the efficiency of solar panels and help eliminate loss due to almost immediate recombination of such carriers. The simulation of these wells required a modeling of the energy band levels of lattice-matched semiconductor heterostructures. The CSUN could then be easily modeled by using a semiconductor material layer in between two layers of a different material with a much larger type 1 energy band gap, where the CSUN layer has a higher valence band, but a lower conduction band level. Therefore, the modeling of the CSUN required an easy yet accurate method for calculating and displaying the energy band lineups for a variety of different semiconductor materials. A screenshot of the final GUI, done in MATLAB, is shown below in Figure 1.



Figure 1. GUI of the heterostructure band lineup modeling

The figure above has many attractive features that make it very effective for such modeling. It can predict the energy bands for a large number of different semiconductor heterostructure combinations. The list of available materials is Si and Ge, the compound

materials of GaAs, AlAs, InAs, GaP, AlP, InP, GaSb, AlSb, and InSb, as well as the alloys of $\text{In}_x\text{Ga}_{1-x}\text{As}$, $\text{Al}_x\text{Ga}_{1-x}\text{As}$, and $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$. When choosing to use an alloy, one can change the percent composition of each of the materials in it, as shown using $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$ below in Figure 2.

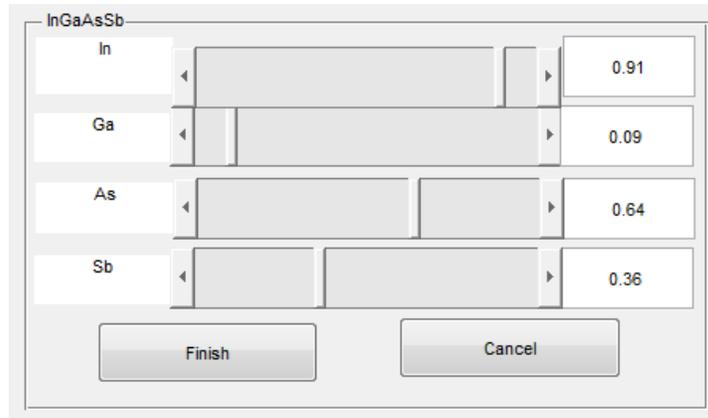


Figure 2. Composition changes of $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{Sb}_{1-y}$

Furthermore, as seen in Figure 1, the GUI also has the option of adding strain to one of the materials, which changes the lattice constant, and thereby also the energy band gap. The material can be strained to the other material's lattice constant along the (001) plane, or by choosing the percent of the change along both the in and out-of plane directions. Finally, the GUI has two plots, for side-by-side comparison of different choices. The plots also contain information such as the energy level differences of the conduction and valence bands between the two materials, ΔE_c and ΔE_v respectively, as well as the band gap of each material.

In order to simulate the behavior of the energy bands in a quick, easily-understood manner, I used the mathematical model of Chris G. van de Walle's Model Solid Theory. This model set the underlying algorithm. First, it predicts the changes that strain will have on the material's parallel and perpendicular lattice constants. Then, from the new lattice constants, it can predict the energy changes in the materials band structure. If multiple bands are present, such as the light-hole and heavy-hole bands in the valence band, the GUI will output the bands which give the lowest energy band gap. In the case of alloys, I used Vegard's Law to find these values, where the value of, for example, the lattice constant is scaled by the percent composition of each of the different alloy materials.

Through the use of the mathematical modeling of van de Walle's theory, I was able to accurately predict the energy band differences of various strained materials. While these are certainly not 100% accurate, they give a basic and reasonable idea of what to expect from such heterojunctions. The GUI is able to efficiently display all the needed information to make an informed decision between several different possible combinations of semiconductor material.

Energy-Efficient Wastewater Treatment Hollow-Fiber Membrane Biofilm Reactors

Sophie Manley
College of Engineering
Civil and Environmental Engineering and Earth Sciences

Advisor: Robert Nerenberg, University of Notre Dame, College of Engineering, Civil and Environmental Engineering and Earth Sciences

Most of wastewater treatment facilities in America use conventional activated sludge (CAS) processes for degrading organic compounds. Generally, CAS system uses traditional air diffuser devices for oxygen supply (aeration) into reaction tanks; these devices have a range between 10 and 40% of oxygen transfer efficiencies (OTE). In addition, energy spent for aeration represent about 60% of the overall amount of energy that a wastewater treatment plant needs, therefore this unitary step represents a key priority process for energy reduction and sustainability studies. The project focused on the improvement of the estimation and prediction of potential energy and economic savings that can be achieved with the implementation of a new advanced technology for aeration, the hollow fiber membrane biofilm reactor (HF-MBfR). This technology is based on biofilm that grows attached to a membrane and can achieve a 100% of OTE. Research has identified several parameters to which energy savings are highly sensitive, and a critical parameter is the removal fluxes. The goal of this research better quantified these parameters. Focusing on a new, polymethylpentene (PMP) membrane, basic properties were determined including the oxygen diffusion coefficient and the fluxes in and out of the biofilm.