



School of Chemical & Biomolecular Engineering

Energy Research



Pradeep Agrawal

Dr. Pradeep Agrawal's research is focused on the development of thermochemical pathways for converting ligno-cellulosic biomass into fuels and chemicals. One approach involves hydrolysis of hemi-cellulose, cellulose, and lignin into monomers which offer an alternate platform for transportation fuels and chemicals. The results offer promise for developing a green chemistry approach so that organic acids derived from the biomass can be utilized for biomass hydrolysis. Another project involves high pressure biomass gasification under conditions that mimic the next generation of gasification processes (short contact times and high heating rates). The aim is to develop mathematical models for high pressure biomass gasification. Gasification offers the advantage that all types of biomass (including agricultural waste and forest residue) can be gasified to produce syngas ($\text{CO} + \text{H}_2$). Biomass gasification involves pyrolysis and char gasification in series. The results have identified the role of heating rates, pressure, alkali metals, and transport effects on biomass gasification.



Thomas Fuller

Dr. Tom Fuller's research addresses challenges in sustainable transportation, specifically lowering emissions of greenhouse gases and reducing dependence on petroleum. Meeting these challenges requires greater use of batteries and other electrochemical devices. Dr. Fuller's research group emphasizes the fundamental causes of degradation in these systems and provides both guidance for the development of new materials as well as system architectures and control strategies to mitigate these failures. This research involves detailed understanding of the mechanisms of performance loss in specific components and is a blend of experiments and physics-based models. For the last couple of years, the emphasis has been on batteries for hybrid-electric and electric vehicles. A prominent application has been power sharing between a fuel cell and battery for a hybrid vehicle. The research has shown that relatively minor changes in control strategies have minimal impact on system efficiency, but dramatically improve life, and therefore life-cycle cost. This research has the potential to fundamentally change the manner in which these systems are designed.



Christopher Jones

Dr. Jones's research group works at the interface of chemistry and chemical engineering, emphasizing the design, synthesis, and application of new materials applied to catalysis, reaction engineering, and separations. The group is composed of predominantly chemical engineering students and postdoctoral researchers but also includes physical, organic, and inorganic chemistry students and postdocs. For the last several years, a growing component of the group's research has been the development of new materials for chemical separations. A particular emphasis has been placed on carbon dioxide capture from dilute gas streams, especially power plant flue gas. Recently, Jason Hicks, PhD ChBE '07 and Jeffrey Drese, PhD ChBE '10 have designed new CO_2 -adsorbing aminosilica materials with large, tunable CO_2 capacities. Today, the group is studying the synthesis-structure-property relationships associated with the new adsorbent materials. The overall goal is to develop a rational framework for the synthesis of adsorbents with precise control of important kinetic and thermodynamic properties such as the rates of adsorption and desorption, the CO_2 capac-





separation platforms that may ultimately lead to more efficient, lower-cost capture of CO_2 from dilute gas streams. Dr. Jones, together with Dr. Sunho Choi, the Dreyfus Postdoctoral Fellow in Environmental Chemistry, Stephanie Didas, a ChBE PhD student, and Dr. Watcharop Chaikittisilp, is also working on the development of adsorbent materials that can efficiently capture CO_2 from ambient air. A technology built on such materials could ultimately lead to a negative carbon technology that could account for emissions from mobile sources such as cars, buses, and planes.

ity, the heat of adsorption, and adsorbent deactivation and stability. A significant emphasis is placed on developing scalable regeneration methods for amine-based sorbents, and generating an understanding of their long-term stability under practical operating conditions, in a study being carried out by PhD student Praveen Bollini. In parallel, Dr. Jones works closely with the Koros and Nair groups on the incorporation of the new adsorbent materials or amine groups into novel



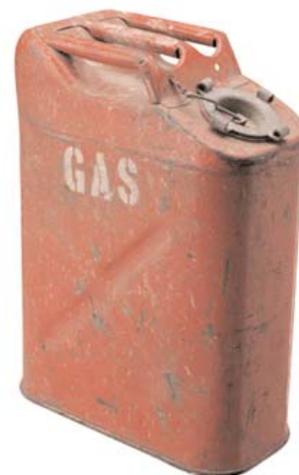
Paul Kohl

Ambient temperature fuel cells hold the potential to be very high-energy, density power sources for portable electronic applications; however, current methanol cells based on proton exchange membranes present many challenges that hinder their utilization, including high cost due to platinum catalysts and high fuel loss. Dr. Paul Kohl's group is exploring a new approach to high-energy-density, low-cost cells based on anionic conducting membranes. Anion-based methanol fuel cells can use non platinum catalysts and high methanol concentrations, including pure methanol feed. The research involves synthesis of new anionic conducting membranes, electrode structures for high catalyst utilization, and system engineering. Research in Dr. Kohl's group has led to the creation of new membranes and ionomers for making electrodes. In addition, the anionic conduction allows new approaches to fuel cell systems. A hybrid design has been created using both cationic and anionic bipolar membranes which self-humidifies the cells, thus reducing the total balance of plant and simplifying the operation. Cells have been operated with external humidity ranging from 0% to 100% relative humidity. The impact of the work includes creating portable power sources with applications for soldiers in the field and similar civilian uses. Methanol would provide a very low-cost and light-weight fuel, lowering the overall size and weight of the power supply. Dr. Kohl's research on anionic conducting membranes is in collaboration with DuPont, Inc.



Ronald Chance

Professor of the Practice Ron Chance holds a joint appointment in ChBE and the School of Chemistry & Biochemistry, a position he assumed after retiring from ExxonMobil in 2006. His main research interests are in CO_2 capture and utilization. However, for the past year and a half, he has spent the majority of his time as executive vice president in charge of engineering for Algenol Biofuels, one of the largest algae-based biofuel companies in the country. In that role, Dr. Chance established a research program at Georgia Tech that involves five research projects and seven professors, including ChBE's William Koros, Chris Jones, Sankar Nair, Matthew Realf, and Victor Breedveld; ISyE's Valerie Thomas; and CEE's Haiying Huang. All of the projects are aimed at analysis and system development related to the commercialization of Algenol's technology for producing ethanol and other chemicals from blue-green algae (cyanobacteria). These projects now form the core of the R&D portion of a \$25 million grant from the Department of Energy (DOE) for building a pilot-scale biorefinery based on Algenol's technology. Other partners in the DOE project are Dow Chemical Company, National Renewable Energy Laboratory (NREL), University of Colorado, and Membrane Technology & Research, Inc. Thus far, research has demonstrated via a state-of-the-art life cycle analysis (LCA) that the Algenol system can deliver a transportation fuel with a carbon footprint up to 80% lower than gasoline, which easily meets the U.S. Renewable Fuels Standard for a renewable biofuel. The work has also produced novel systems for gas management (CO_2 , O_2 , ethanol) in photo-bioreactors. Although this research focuses on the Algenol system, there is demonstrated potential for broad applicability to algae-to-fuels technologies. Additionally, two Algenol scientists who are in residence at Georgia Tech are working on synergistic projects. This partnership has benefited enormously from financial support from the Georgia Research Alliance in the formative stages of the program.





William Koros

Dr. Koros focuses on efficient large-scale separation and purification processes. His non-traditional approach relies upon membrane and sorption separators that can reduce both energy consumption and CO₂ emissions by as much as a full factor of ten for each unit of product produced. Natural gas for energy production is available; however, it is not currently purified in energy-efficient processes. Moreover, after production, downstream processing of natural gas and other hydrocarbons for fuels and valuable chemical

products occurs in energy-intensive inefficient complexes. Dr. Koros combines materials science and separations science to create hollow fiber units with diameters the size of a human hair to molecularly separate complex mixtures in diverse processes to improve these processes. Bundles of these fibers can provide more than two football fields worth of separation area in compact modules smaller than an office desk. Their compact nature makes membrane modules attractive for off-shore applications where available space is scarce. Besides membranes, Dr. Koros has expanded his work to create fiber sorbent modules to precisely capture contaminants such as mercaptans, low pressure CO₂, or ethanol from large but dilute feed streams. The engineering of such separation devices combines cross-cutting elements of traditional chemical engineering, nanotechnology, and materials chemistry to address problems of major relevance to energy production, economic development, and environmental sustainability.



David Sholl

Developing new technologies to make large-scale carbon capture economically feasible will require breakthroughs in materials and processes, not just incremental advances on existing technologies. The risk in developing any new class of materials is high, so the ability to make useful predictions about materials properties without undertaking time-consuming experimental studies can be crucial in jump-starting work in a new area. Dr. Sholl's group uses detailed computational modeling methods to accelerate the search for new materials in applications where the number of possible materials is too large to be considered by traditional experimental testing. Many of the applications his group focuses on are directly driven by the development of carbon capture technologies or emission-

reduction processes. For example, his group uses efficient computational methods to examine nanoporous zeolites and metal-organic frameworks for use as membranes for carbon dioxide separations. The models, which begin with atomically detailed structures for each material, allow researchers to consider hundreds of candidate materials and refine this diverse group into a small number of the most promising candidates. In another example, Dr. Sholl's group is using similar approaches to develop metal alloy films that can economically produce ultra-high-purity hydrogen from the high-temperature syngas mixtures that are relevant in gasification processes. This purification process, if implemented on large scales, could play a key role in using existing hydrocarbon resources in a carbon-neutral way. These computational efforts are strongly coupled with experiments being performed by Georgia Tech colleagues and external collaborators.



Sankar Nair

A significant component of Dr. Nair's research addresses problems in environmentally benign processing and utilization of materials, chemical feedstocks, and fuels. This research involves the engineering of advanced materials and membranes, as well as fundamental studies of structure-property relationships in these (usually nanostructured) materials and membranes. Some prominent applications include the removal of greenhouse gases and acidic or toxic impurities from gaseous fuels, economical separation of biofuels such as ethanol from aqueous feed streams, development of better membranes for potential use in fuel cell devices, and environmentally benign processing of new functional materials to be incorporated in nanocomposite films and membranes for a

variety of technological applications. A common scientific theme uniting these research problems is the challenge of tailoring and functionalizing the structure, shape, composition, and architecture of materials and membranes in a rational manner to achieve high performance in the desired applications. This research program enjoys substantial collaborations with the research groups of Drs. Chris Jones, William Koros, and David Sholl. Several aspects of this program involve a unique synergy of experimental and computational research in order to create a strong scientific foundation for the pursuit of technological advances. It also benefits from the support and collaboration of industrial, federal, and other organizations. Approximately a dozen PhD-track, MS-track, and postdoctoral researchers are pursuing this work. A number of ChBE undergraduate students, as well as high school teachers in the Atlanta area, have also taken advantage of the substantial research and hands-on educational opportunities created by this program.



Rachel Chen

Dr. Rachel Chen and her research group focus on engineering microbial biocatalysts for conversion of cellulose and hemicelluloses into biofuels molecules. While there now exist many natural and engineered microbes that readily convert monomer sugars into biofuels (e.g., butanol), they are typically unable to use polymeric sugars. Consequently, additional process steps are needed, including pretreatment, enzyme production, and enzymatic de-polymerization, adding significant costs to the process. A radically different approach known as “consolidated bioprocessing” aims to simplify the process by combining all these steps into one. However, microbes capable of turning cellulose into biofuel in a single step (in a single reactor) have yet to be developed. Dr. Chen’s research group is applying metabolic engineering and synthetic biology to create such catalysts. They mix and match “biological parts” functioning as “transporter,” “sugar-depolymerizer,” and “biofuel-synthesizer” from different microorganisms and eventually integrate these parts into one microbe that is capable of multitasking as required in a consolidated bioprocess.



Matthew Realf

Dr. Matthew Realf’s research focus is sustainable systems engineering, which has emerged as an important interdisciplinary topic between engineering and both physical and social sciences. He works on developing processes to make fuels from trees and crops, as well as analyzing supply chains that start with plants or trees in the field, convert them into fuels, and distribute the fuels to end use customers. For example, graduate student Korin Reid is building models to study the interaction of biofuel systems with climate change. To advance this topic, Dr. Realf is working with Tony Giarrusso and Dr. Steve French of the Geographic Information Systems Center and ChBE’s Dr. Athanasios Nenes and Earth and Atmospheric Science professor Dr. Armistead Russell. For this project, computationally intensive climate-change models are coupled with models that can predict how altered rainfall, temperature, and sunlight impact crop yields. The long-term goal of this project is to create biofuel systems that do not negatively impact climate change by increasing land use change in an effort to maintain fuel production.



Michael Filler

Dr. Michael Filler’s research program lies at the intersection of chemical engineering and materials science, emphasizing the scientific and engineering challenges that currently limit widespread deployment of solar power generation. This research leverages properties inherent to the nanoscale to create custom-designed light harvesting materials, particularly semiconducting nanowires. The majority of this work comprises two important research thrusts: (1) prototyping novel materials and photovoltaic device nanoarchitectures and 2) fundamentally interrogating nanomaterials during the fabrication process. More specifically, the ability to tune atomic composition beyond what is possible in the bulk is being utilized to create earth-abundant and non-toxic alloy nanowires with the potential to capture photons from across the solar spectrum. The study of model nanowire systems with in-situ spectroscopic techniques is providing an atomic-scale understanding of the bulk and surface chemistry that dominates nanowire photophysics. Through these studies, Dr. Filler’s group is gaining the knowledge and synthetic control necessary to realize ultra-high-efficiency and simultaneously scalable solar cell technologies.



Athanasios Nenes

Dr. Nenes’s research focuses on atmospheric particles and understanding their impacts on air quality, clouds, radiation, and climate. His research is driven by the need to obtain predictive understanding of the impacts humans have (especially those associated with energy production/consumption) on the environment. The research group is engaged in a diverse set of multiscale modeling and experimental efforts. One effort focuses on developing computationally efficient and comprehensive aerosol thermodynamic models (ISORROPIA, ISORROPIA-II) for use in regional and global atmospheric models such as the EPA Community Model for Air Quality, the CAMx aerosol model, the Harvard GEOS-

CHEM, the Meteo-France Polyphemus, and the Max Plank GMEx model. His group is also involved in developing and commercializing instrumentation for fast and highly accurate measurements of the cloud-droplet-nucleating characteristics of atmospheric particles, as well as devising comprehensive indirect techniques for characterizing organic-water interactions and hygroscopicity of organic compounds found in particulate



matter. Another aspect of Dr. Nenes's research involves laboratory studies and ground-based and airborne field studies on cloud condensation nuclei (CCN) activity and aerosol-cloud interactions. His group is also engaged in the modeling of aerosol-cloud-climate interactions and is working on developing and evaluating cloud microphysical parameterizations for use in numerous regional and global climate models used in the US and Europe. Finally, Dr. Nenes's group is studying the impacts of marine ecosystem productivity on clouds and climate, as well as the effects of air pollution on oceanic iron bioavailability.



Carsten Sievers

Dr. Carsten Sievers's research group develops catalytic processes for the production of fuels and chemicals from biorenewable resources. A biomass-based economy presents new challenges for catalysts because the reactants are more complex than oil-derived compounds, and little is known about their interaction with solid catalysts. Dr. Sievers's research group addresses these issues by developing spectroscopic techniques to identify surface-bound intermediates and their reaction pathways. In combination with detailed characterization of the catalysts, these studies provide design criteria for new selective catalysts for the production of specific chemicals and fuels. In parallel, Dr. Sievers's group improves the stability of solid catalysts in water, which serves as the medium in many processes for biomass conversion. In addition to these fundamental studies, his research group also develops specific catalytic processes for upgrading of pyrolysis oils, conversion of glycerol to value-added chemicals, and production of biofuels via gasification. The combination of fundamental and applied studies enables novel processes for future biorefineries.



Krista Walton

The selective removal of CO₂ from nitrogen-containing streams such as flue gas or methane-containing streams such as natural gas is one of the grand challenges for separations science. Conventional porous materials such as zeolites and activated carbons often have low selectivities and are difficult to regenerate, which leads to significant expense. Metal-organic frameworks (MOFs) represent a new direction in porous materials research that could lead to the creation of designer-specific multifunctional materials. The rich field of coordination chemistry provides a versatile platform from which these materials may be assembled from an almost infinite set of building blocks. In contrast to conventional microporous materials, these hybrids are formed through interconnection of metal clusters and organic ligands. They have demonstrated interesting adsorption properties and have a clear potential for impacting a wide range of adsorption-based technologies. Metal sites can be coordinatively unsaturated and exposed on the interior surfaces of the material where they are open to direct approach by sorbate molecules. The organic ligand used to construct the material can be functionalized in a variety of ways. Thus, a material may be synthesized with open metal centers and pore walls decorated with various functional groups to provide molecule-specific binding sites. The goal of Dr. Walton's work is to manipulate MOF chemistry to create novel metal-organic structures with regenerable CO₂-specific adsorption sites. Her group's strategy focuses on developing methods to synthesize MOFs through assembly of the paddle-wheel structure using copper atoms and by functionalizing the organic ligand with amine groups. This research has the potential to open a completely untapped class of materials to the development of new and improved adsorbents for selective and efficient CO₂ capture.



Andreas Bommarius

Dr. Andreas Bommarius's research focuses on the development of new functional proteins and the improvement of existing ones. In the hydrolysis of (ligno)cellulosics to glucose, the action of the enzyme exo-cellobiohydrolase 1 (CBH 1) is the rate-limiting step. CBH 1 has to adsorb on the cellulose surface, loosen the cellulose fiber, thread the fiber from one domain (the cellulose-binding domain) into a tunnel-like structure en route to the active site in the catalytic domain. The Bommarius lab works to improve the overall effectiveness of CBH 1 and its components, especially in cellulose of moderate and high levels of crystallinity. Key results include the demonstration of jamming—the mutual hindering of cellulase enzyme molecules—as the cause of the rate slowdown at high conversion of cellulose and the use of binding domains (CBDs) as a form of biological pretreatment. Current challenges focus on finding a comprehensive kinetic model for lignocellulose hydrolysis and on finding effective ways of lowering the degree of crystallinity without the usual chemical pretreatment.

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