Sustainable Energy Research and Education at the University of Notre Dame

Professor Joan Brennecke
Keating Crawford Professor of Chemical and Biomolecular Engineering and Director, SEI

Professor Ken Henderson
Professor and Department Chair, Chemistry and Associate Director, SEI

Patrick Murphy
Managing Director, SEI
The technologically advanced societies can and must lower their domestic energy consumption, either through an evolution in manufacturing methods or through greater ecological sensitivity among their citizens. It should be added that at present it is possible to achieve improved energy efficiency while at the same time encouraging research into alternative forms of energy.

- Pope Benedict XVI
Safer Nuclear

Cleaner Fossil

Advanced Solar

Optimal Wind

Efficient Use
• In the near term, we will continue to use coal and gas for electricity and petroleum for transportation.
• But we will need and can achieve more environmentally responsible methods of using these resources.
• Managing CO₂ emissions will be key.
Cleaner Fossil Research at ND

- CO$_2$ Capture, Conversion, Sequestration
- Catalysis
- Computation
- Combustion
- Systems Dynamics, Process and Economic Modeling
CO$_2$ Capture, Conversion, Sequestration
Joan Brennecke

- Keating-Crawford Professor of Chemical and Biomolecular Engineering
- Director, Notre Dame Energy Center
- Director, Sustainable Energy Initiative
- jfb@nd.edu

**Capabilities**

**Gas Uptake**
- Stoichiometric apparatuses
- Gravimetric microbalances (Hiden IGA, Rubotherm)

**In-situ Fourier Transform Infrared (FTIR)**

**Vapor-Liquid Equilibria (VLE)**
- Head space Gas Chromatograph (GC)
- Cottrell pump re-circulating still

**Calorimetry**
- Solution calorimeters Setaram C80 and microDSC III
- Mettler Toledo DSC

**Decomposition**
- Mettler Toledo TGA
- Varian GC/Mass Spectometer (GC/MS)

**Viscometers (parallel plate and cone & plate)**

**Vibrating tube densitometers**

**Liquid Liquid Equilibria (LLE)**
- High Performance Liquid Chromatography (HPLC)
- GC
  - Ultraviolet and visible (UV-vis) spectroscopy

**Potential Coal Research**

- Thermodynamic measurements of OTHER materials (e.g., adsorbents)
- ILs for other things
  - Electrochemical/photochemical conversion of CO₂ (high solubility, good conductivity, etc.)
  - Actinide separations
    - Electrochemical separation using IL as medium
    - Solubility of various oxides in ILs
    - Radiolysis of ILs
  - Precombustion flue gas separations (from gasification)

**Current Energy Research**

**CO₂ Capture**

**Refrigeration Systems**

**Liquid Separations**

- Gurkan et al., JACS, 2010
Kenneth Henderson

• Professor and Department Chair of Chemistry and Biochemistry
• Associate Director, Sustainable Energy Initiative
• khenders@nd.edu

Capabilities
Inorganic synthesis and characterization
Organometallic s-block chemistry
  • (Li—Cs, Mg—Ba)
  • organic methodology development
Metal-organic frameworks
Solution structure and dynamics
Solid-state structure
Basic user of theory (DFT)

Current Energy Research

Metal-Organic Framework Applications

- Selective Guest Uptake:

- Postsynthetic Covalent Modification:

- Gas Purification:

- Gas Sorption:

Potential Coal Research

• MOFs for CO₂ sequestration or gas purification – measurements
• Supported catalysis on high surface area materials – catalysis / measurement

Geminal Dianions: R₂CM₂ M=Li, Na, K
Capabilities

Carry out atomistic-based simulations to compute properties of materials (Monte Carlo, molecular dynamics, coarse-grained)
  - Phase equilibria (VLE, LLE, SLE, etc.)
  - Thermodynamic properties (heat capacity, density, expansivity, etc.)
  - Transport properties (viscosity, conductivity, diffusivity, mass transfer)
  - Insight (fluid structure, explain behavior, etc.)

Develop new simulation methods
  - Melting points
  - Advanced free energy calculations
  - Nonequilibrium molecular dynamics

Develop predictive force fields using \textit{ab initio} simulations

Systems of interest
  - Liquids, crystalline materials, nanoporous materials

Current Energy Research

Ionic liquids
  - CO\textsubscript{2} capture (DOE NETL with JFB, WFS, MJM)
  - Geothermal and absorptive cooling (DOE with JFB et al.)
  - Solar thermal / enhanced with nanoparticles (DOE with SRNL and USC)
  - Hypergolic fluids and electropropulsion (AFOSR, with Hanscom AFB, UC Berkeley)
  - Structure and properties at electrode interfaces (Sandia NL)

Actinides
  - Simulation of uranyl and other actinyl species (EFRC)

Method development
  - Expanded ensemble MC for solvation modeling
  - Melting point and polymorph stability prediction

Potential Coal Research

Looking for experimental collaborators who could use insights gained from molecular simulation

Types of experimental probes
  - “Bulk” properties (thermodynamic, transport properties)
  - “Molecular” properties (spectroscopy, single molecule imaging)

Potential areas
  - H\textsubscript{2}/CO\textsubscript{2} separation
    - sorption and diffusion in nanoporous materials (MOFS, membranes)
  - Ionic conductivity in IIs
    - Mechanism of conduction
  - Behavior of confined IIs in separation applications (SILMs)
    - PFG NMR, single-molecule probes of IIs confined in nanopores
    - Bulk sorption behavior

Edward Maginn

- Professor of Chemical and Biomolecular Engineering
- Graduate School Associate Dean of Academic Programs
- ed@nd.edu
Chongzheng Na
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Website: www.nd.edu/~cna and email: cna@nd.edu

Current Energy Research
Elucidate the physicochemical origins of chalk-pore hydrophobicity to improve oil-recovery efficiency

Capabilities
• Experimental interrogation of interfacial physics and chemistry using advanced scanning probe microscopy
• Elucidation of molecular mechanisms of surface and interfacial reactions

Reduce energy loss of coal from weathering during mining, transportation, and storage

Potential Coal Research
• CO$_2$ sequestration in coal seams
• Underground coal gasification
• Resource recovery from syngas wastes
Bill Phillip

• Assistant Professor of Chemical and Biomolecular Engineering (Fall 2011)

Capabilities

• Fabricating and characterizing thin-film composite membranes for forward osmosis applications, using phase inversion and interfacial polymerization protocols
• Modeling and establishing experimental procedures to confirm the predictions of the model for reverse diffusion of draw solutes in forward osmosis operations
• Producing novel ultrafiltration, nanofiltration, and osmosis membranes that use new classes of nanomaterials including nanoionic materials (NIMs) and block polymers

Current Research

Simultaneous Reaction and Separation Can Improve Process Efficiency. 1) equilibrium limited reactions, 2) reactions producing an inhibitor, and 3) series reactions with a desirable intermediate product.

Potential SEI Research

• Use of materials science to engineer novel separation systems like membranes and adsorbents
  • Porous reactive membranes capable of degrading emerging contaminants
  • Charge mosaic membranes that separate salt from water
  • Cyclic separating reactors that improve process performance by combining separation and reaction
**William Schneider**

- Professor of Chemical and Biomolecular Engineering
- Professor of Chemistry and Biochemistry
- wschneider@nd.edu

**Capabilities**

- First Principles Simulations
  - structures and thermodynamics
  - Reaction rates
  - Reaction dynamics
- Catalytic and Environmental Reaction Simulation
  - Environmental effects on surface kinetics
  - Fundamentals of surface catalytic reactions

**Current Research**

**Atomic scale simulation**, based on *Density Functional Theory*

**Specific Areas of Research**

- Ionic Liquids for CO₂ Capture
- Catalytic NO oxidation
- Water gas shift
- Catalytic NO reduction
- Perovskite catalysis

**Structures & thermodynamics**

**Reaction Rates**

**Reaction dynamics**

**Potential Coal Research**

Collaboration on site-specific/homogeneous energy-related catalysis
**Capabilities**

Synthesis and Characterization:
- Design and multistep synthesis of complex organic ligands
- Synthesis of soluble discrete inorganic organometallic compounds
- Characterization (NMR, IR, MS, CD, UV-Vis, X-ray, electrochemistry)
- Pedestrian electronic structure calculations

Mechanistic Study:
- Kinetics by NMR, UV-Vis
- Dynamic NMR
- Isotopic labeling/isotope effects
- Structure-activity relationships

**Electrocatalysis via Redox-Active Ligands**

Four steps
53% overall yield

**Potential Coal Research**

Dioxygen Activation/Production
- High coordination numbers and high redox capacity to stabilize (or bypass) peroxide intermediates

Carbon Dioxide Activation by Novel Mechanisms
- Hydride transfer from redox-active ligands/metal hydroxides?
- Organoelectrocatalysis?
Current Energy Research

- Chemical, electrochemical and photochemical catalysis in the degradation of lignin
- Catalytic dechlorination reactions
- Preparation of new heteropolymetallate-organic framework materials for photochemical redox catalysis
- Polymeric materials with tethered tetraaza-macrocyclic complexes for photochemical and electrochemical catalysis

Potential Coal Research

- Degradation of lignin for efficient biofuel production
- New materials for CO₂ reduction

Capabilities

- Electrochemical Analysis
- Rapid kinetic analysis
- Kinetics and mechanism of thermal and photochemical reactions

Inorganic Reaction Mechanisms

Spectra of aerated solutions containing lignin and poly(HOAlIIItspc) before and after a 5 h (λ > 500 nm) irradiation, dotted lines, and the lignin alone (solid line). Inset: average structure of poly(HOAlIIItspc).
Catalysis
Seth Brown

• Associate Professor of Chemistry and Biochemistry
• sbrown3@nd.edu

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Potential Coal Research
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- Associate Director, Sustainable Energy Initiative
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- Metal-organic frameworks
- Solution structure and dynamics
- Solid-state structure
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**Current Energy Research**

**Metal-Organic Framework Applications**

- **Selective Guest Uptake:**

- **Postsynthetic Covalent Modification:**

- **Gas Purification:**

- **Gas Sorption:**

**Potential Coal Research**

- MOFs for CO₂ sequestration or gas purification – measurements
- Supported catalysis on high surface area materials – catalysis / measurement

**Geminal Dianions:** $R_2CM_2$ \( M=\text{Li, Na, K} \)

**Organometallic and Supramolecular Synthesis**

**Magnesium-mediated synthesis**

**Metal-organic frameworks**
Current Energy Research

Synthesis of novel nanostructures of transition metal chalcogenides
- Aqueous, low temperature (< 100°C), chemical bath deposition synthesis of ZnS, ZnSe, CdS, and CdSe nanoparticles
- ZnS and CdS nanofibers using 1-adamantanethiol as growth modifier

Potential Coal Research

Cleaner Fossil Fuel Processes Thrust *
- NSF CMMI Tribology and Surface Chemistry of Metal Diboride Single Crystals – submitted 10/1/09 $312,522 (still pending)
- Synthesis and characterization of anti-sintering metal nanoparticle - metal-oxide supported heterogeneous catalysts – use of buffer-layer assisted growth of metal nanoparticles on metal-oxide supports
- Novel synthesis and tribological characterization of layered transition metal chalcogenides – thin films or lubricant formulation additives of MoS2, MoSe2, WS2, WSe2, and VS2, VSe2 nanostructures

*Since 1980, reducing friction in automotive components has led to an increase in average fuel economy from 20 to 25 mpg, despite average horsepower doubling from 100 to 190 (New York Times, March 30, 2006)
Potential SEI Research

• Catalyst development and screening for biofuels production from lignin
• Advanced biofuels from cellulosic degradation products
• Synthesis and characterization of hydrodeoxygenation catalysts
• Synthesis of organic / inorganic hybrid materials for CO₂ capture

CDS High Pressure Pyrolysis with Reactor in-line with Agilent GC/MS

Capabilities

Synthesis of organic / inorganic hybrid materials
• Schlenk lines

Synthesis of microporous and mesoporous inorganic oxides
• Synthesis ovens
• Calcination ovens
• Reactor bombs

Pyrolysis of biomass and biomass-related model compounds
• High pressure pyrolyzer
• In-line catalytic reactor
• In-line GC/MS for product analysis

High pressure / high temperature catalytic reactions
• High pressure / high temperature Parr reactor
**Potential Coal Research**

- Synthesis of a novel catalyst for effective CO₂ conversion
- Dynamic methods for coal combustion investigation
- Kinetics of coal combustion reactions
- Microstructural aspects of coal combustion

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**Current Energy Research**

**Combustion of Heterogeneous Nanostructural Systems**

**Capabilities**

**High Speed Infra Red Thermo Vision System**
- Temperature range 300-2300 K
- Time resolution up to 0.1 ms
- Space resolution 10 microns

**Combustion Reactor**
- Volume 3 liters
- Gas pressure up to 100 atmosphere
- Temperatures up to 3000 K

**High Energy Ball Milling** PM100 Planetary Ball Mill
(Retsch GmbH, Germany)
- Rotation speed up to 650 rpm
- Inert or reactive gas atmosphere

**Kinetics of Heterogeneous Reactions** ETA analyzer
(ALOFT, Berkeley, CA)
- Time resolution 0.1 ms
- Temperature range up to 3000 K

**Characterization of Material Microstructure**
- FESEM, Magellan 400 (FEI, USA), resolution 0.5 nm
- EDX and STEM capabilities
- Nano laboratory Helios 600
Franklin (Feng) Tao

**Capabilities**

Synthesis of Nanocatalysts;  
Operando studies of surface chemistry of catalysts;  
High pressure scanning tunneling microscopy of catalysis studies;  
• Surface structure of catalysts at atomic level under reaction conditions  
• Simultaneous measurement of catalytic activity and selectivity  
Ambient pressure X-ray photoelectron spectroscopy of catalysis studies;  
• Surface composition, oxidation state, and restructuring  
• Identification of active catalytic phase  
• Simultaneous measurement of catalytic activity and selectivity.  

Catalysis in environmental remediation;  
Catalysis in solar chemistry;  
Catalytic measurements of ambient pressure reactor and high pressure reactor.  

Available instruments in Tao group:  
ambient pressure XPS and high pressure STM

**Current Energy Research**

1. Surface structure of catalysts under reaction conditions  
2. Surface chemistry of catalysts under reaction conditions  
3. Operando study of fuel cell processes  
4. Operando study of Solar chemistry

**Potential Coal Research**

• Synthesis of Fisher-Tropsch catalysts by nanoscience  
• Evolution of surface structure of catalysts under reaction conditions  
• Identification of active catalytic phase of Fisher-Tropsch reaction  
• Develop F-T catalysts with high selectivity  
• In-situ surface chemistry in the processes of utilizing coal.

**Tenure track assistant professor**  
Department of Chemistry and Biochemistry,  
Department of Chemical and Biomolecular Engineering  
University of Notre Dame  
**Visiting scientist**  
Notre Dame Radiation Lab, DOE  
**ftao@nd.edu**  
**http://www.nd.edu/~ftao**

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**Current Energy Research**

1. Surface structure of catalysts under reaction conditions

10⁻¹⁰ Torr  10⁻⁷ Torr  10⁻¹ Torr

2. Surface chemistry of catalysts under reaction conditions

3. Operando study of fuel cell processes

4. Operando study of Solar chemistry

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**Potential Coal Research**

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- Professor of Chemistry and Biochemistry
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Current Research

Atomic scale simulation, based on Density Functional Theory

Potential Coal Research

Collaboration on site-specific/homogeneous energy-related catalysis

Specific Areas of Research

- Ionic Liquids for CO₂ Capture
- Catalytic NO oxidation
- Water gas shift
- Catalytic NO reduction
- Perovskite catalysis
Eduardo Wolf

• Professor of Chemical and Biomolecular Engineering
• ewolf@nd.edu

Capabilities

• High throughput synthesis and preparation
• Parallel activity evaluation and parallel operando spectroscopy
• Kinetics simulation

Current Energy Research

• Catalysis
• Novel Impregnated Layer Combustion Synthesis (ILCS) with Alex Mukasyan (NSF CBET 0730190)
• Cu/ZnO/ZrO2-Pd catalyst for H₂ production from the oxidative reforming of methanol/ethanol. (US Patent 7,659,227, 2010)
• Hypothesis: Catalytic activity can be modified by applying external voltage to metal – support junction
• Pt nanowires prepared by e-beam lithography ANL
• A new IR enhance reflectance technique developed to study adsorption on small surface areas (1 mm²)
• DFT computational studies (W. Schneider) of the effect of an external electrical field on adsorption
• Verified chemicurrent during CO oxidation

Potential Coal Research

• Clean fossil fuels: ILCS of high area
• Fe-Co oxides for FT synthesis.
Computation
Steven Corcelli

- Assistant Professor of Chemistry and Biochemistry
- scorcell@nd.edu

Capabilities
- Theoretical and computational chemistry
  - Molecular dynamics
  - Quantum chemistry
  - Spectroscopy theory
- Spectroscopic probes of biomolecular hydration, structure, and dynamics
- Modeling reactivity at aqueous/solid interfaces
- Charge transfer in confined environments

Potential Coal Research
- Ab initio molecular dynamics (AIMD) simulations of electrons solvated in NH₃ (collaboration with NDRL)
- Development of adaptive quantum mechanics/molecular mechanics (QM/MM) methods for studying reactivity at liquid/solid interfaces

Current Energy Research
- Computer simulations of aqueous metal oxide interfaces
  Collaboration with Bill Schneider and Kathie Newman
- Nonadiabatic charge transfer in the condensed-phase

DNA hydration and damage
Infrared probes of biomolecular dynamics
J. Daniel Gezelter
Associate Professor of Chemistry and Biochemistry
Director of Graduate Admissions
gezelter@nd.edu

Capabilities
Theoretical & Computational Chemistry
Molecular Dynamics
Phase transitions
Non-equilibrium Dynamics
Simulation Methodologies:
• Fast electrostatics
• Non-equilibrium MD
• Langevin Dynamics, NPT-LD

Lipid Bilayers:
• Molecular-scale modeling of lipid phase behavior

Water & Ice:
• Thermodynamics of insect anti-freeze protein (AFP) binding to ice
• Novel ice polymorphs
• Ion migration in thermal gradients

Metals & Nanoparticles:
• Models for metal–capping agent and metal–water interactions
• Particle-to-solvent thermal transport
• Alloying and de-alloying in bimetals

Current Energy Research

Metals & Nanoparticles:
• Pressure-induced metastable phase-separation in Pd/Pt bimetallic particles [Constant pressure Langevin hull, NEMD]

Water:
• Ion pair separation in thermal gradients [RNEMD]

 Potential Coal Research
• Fluctuating density force fields for classical simulation of molecule-to-metal surface interactions [corrosion & catalysis]
• Better water models for high temperature and pressure conditions [supercritical H2O reactors]
• Reactive bond-order force fields [chemistry]
Potential Coal Research

Looking for experimental collaborators who could use insights gained from molecular simulation

Types of experimental probes

- “Bulk” properties (thermodynamic, transport properties)
- “Molecular” properties (spectroscopy, single molecule imaging)

Potential areas

- H₂/CO₂ separation
  - sorption and diffusion in nanoporous materials (MOFS, membranes)
- Ionic conductivity in IIs
  - Mechanism of conduction
- Behavior of confined IIs in separation applications (SILMs)
  - PFG NMR, single-molecule probes of IIs confined in nanopores
  - Bulk sorption behavior

Capabilities

Carry out atomistic-based simulations to compute properties of materials (Monte Carlo, molecular dynamics, coarse-grained)
- Phase equilibria (VLE, LLE, SLE, etc.)
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- Insight (fluid structure, explain behavior, etc.)

Develop new simulation methods
- Melting points
- Advanced free energy calculations
- Nonequilibrium molecular dynamics

Develop predictive force fields using ab initio simulations

Systems of interest
- Liquids, crystalline materials, nanoporous materials

Current Energy Research

Ionic liquids
- CO₂ capture (DOE NETL with JFB, WFS, MJM)
- Geothermal and absorptive cooling (DOE with JFB et al.)
- Solar thermal / enhanced with nanoparticles (DOE with SRNL and USC)
- Hypergolic fluids and electropropulsion (AFOSR, with Hanscom AFB, UC Berkeley)
- Structure and properties at electrode interfaces (Sandia NL)

Actinides
- Simulation of uranyl and other actinyl species (EFRC)

Method development
- Expanded ensemble MC for solvation modeling
- Melting point and polymorph stability prediction

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• Graduate School Associate Dean of Academic Programs
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Karel Matouš

- Associate Professor of Aerospace and Mechanical Engineering
- Director of Computational Physics Laboratory
- kmatous@nd.edu

Capabilities and Facilities
- Chemo-Thermo-Mechanical Parallel Solver
- Fluid-Structure Interactions
- Micro-CT Imaging and In-situ testing
- Statistical Characterization of Material's Morphology
- High-performance Parallel Computing

Current Research
- Computational Mechanics and Physics
- Computational Materials Science
- Multi-scale/Multi-time/Multi-physics Modeling of Complex Heterogeneous Systems
- Microtomography-based Computational and Experimental Modeling of Heterogeneous Materials

Potential Coal Research
- Material Characterization and Statistical Learning
- Chemo-Thermo-Mechanical Modeling

Propellant Combustion
William Schneider

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- Professor of Chemistry and Biochemistry
- wschneider@nd.edu

Capabilities

- First Principles Simulations
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  - Reaction rates
  - Reaction dynamics
- Catalytic and Environmental Reaction Simulation
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  - Fundamentals of surface catalytic reactions

Structures & thermodynamics

Coverage-dependent activation energies

\[ \text{Phys. Rev. Lett. 2009, 102, 076101} \]

Anion vs. Cation Tethered Amines for CO\(_2\) Capture

\[ \text{ACS Symposium Series, 2010} \]

Atomic scale simulation, based on Density Functional Theory

Specific Areas of Research
- Ionic Liquids for CO\(_2\) Capture
- Catalytic NO oxidation
- Water gas shift
- Catalytic NO reduction
- Perovskite catalysis

Current Research

Reaction Rates

\[ \text{CI-NEB} \]

Reaction dynamics

Potential Coal Research

Collaboration on site-specific/homogeneous energy-related catalysis
Potential SEI Research

- General Computational Support
  - Geometric & electronic structures
  - Properties of small molecules
  - Force field generation
- Clean Fuel Initiatives
  - Reaction pathways & intermediates
  - Catalyst design

Current Energy Research

- Electron Transfer
  - Solar energy conversion,
  - Molecular electronics
- Reaction Mechanisms
  - Kinetics and thermodynamics
  - Reaction pathways
- Homogeneous Catalysis
  - Transition metal catalysis
  - Ligand design

Capabilities

- Electronic Structure Calculations
  - DFT, HF, post HF
  - Solvent models
- Multiscale Modeling
  - Quantum Guided MM (Q2MM)
  - Reaction pathways
- Molecular Design
  - Property predictions
  - Design & synthesis of small molecules

\[ y = 0.9854x - 0.0452 \]
\[ R^2 = 0.9572 \]