SEI Faculty

1. Joan Brennecke
2. Seth Brown
3. Bruce Bunker
4. Steven Corcelli
5. Luis Fernandez-Torres
6. J. Daniel Gezelter
7. Gregory Hartland
8. Kenneth Henderson
9. Jason Hicks
10. Prashant Kamat
11. Masaru Kuno
12. Jay LaVerne
13. Edward Maginn
14. Paul J. McGinn
15. Chongzheng Na
16. Bill Schneider
17. Mark Stadtherr
18. Franklin Tao
19. Olaf Wiest
20. Eduardo Wolf
21. Thomas Albrecht-Schmitt
22. Peter Burns
23. Ian Carmichael
24. Jeremy Fein
25. Graham Lappin
26. Slavi Sevov
27. Mark Wistey
28. Zhiliang Xu

Joan Brennecke

- Keating-Crawford Professor of Chemical and Biomolecular Engineering
- Director, Notre Dame Energy Center
- Director, Sustainable Energy Initiative

Capabilities

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

In-situ Fourier Transform Infrared (FTIR)

Vapor-Liquid Equilibria (VLE)
- Head space Gas Chromatagraph (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)

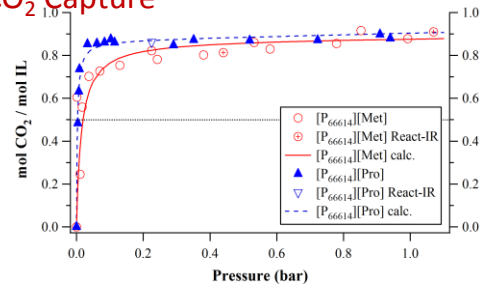
Vibrating tube densitometers

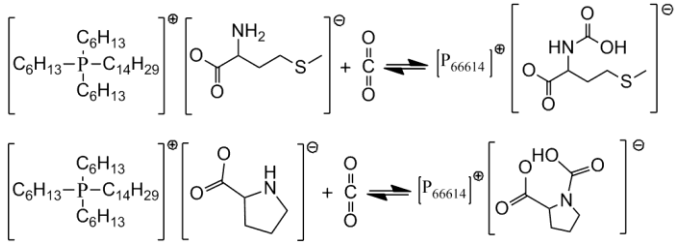
Liquid Liquid Equilibria (LLE)
- High Performance Liquid Chromatography (HPLC)
- GC
- Ultraviolet and visible (UV-vis) spectroscopy

Process demonstration

Current Energy Research

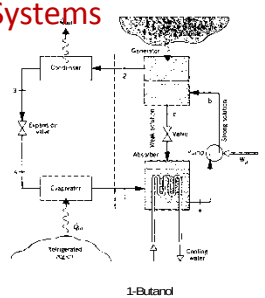
CO_2 Capture



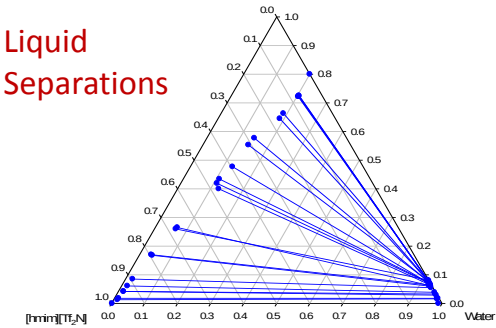


Gurkan et al., JACS, 2010

Refrigeration Systems



Liquid Separations



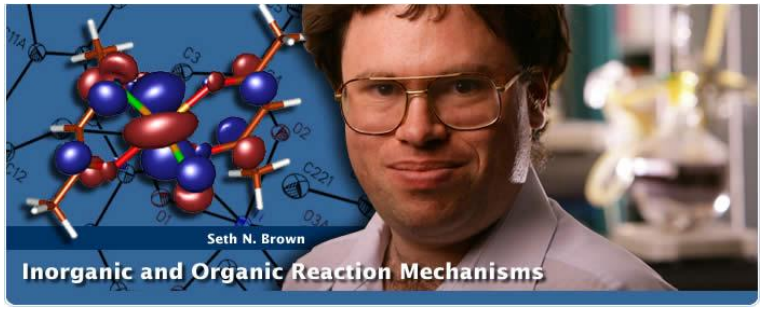
Potential SEI Research

Thermodynamic measurements of OTHER materials (e.g., adsorbents)

ILs for other things
- Electrochemical/photochemical conversion of CO_2 (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)

Seth Brown

- Associate Professor of Chemistry and Biochemistry



Capabilities

Synthesis and Characterization:

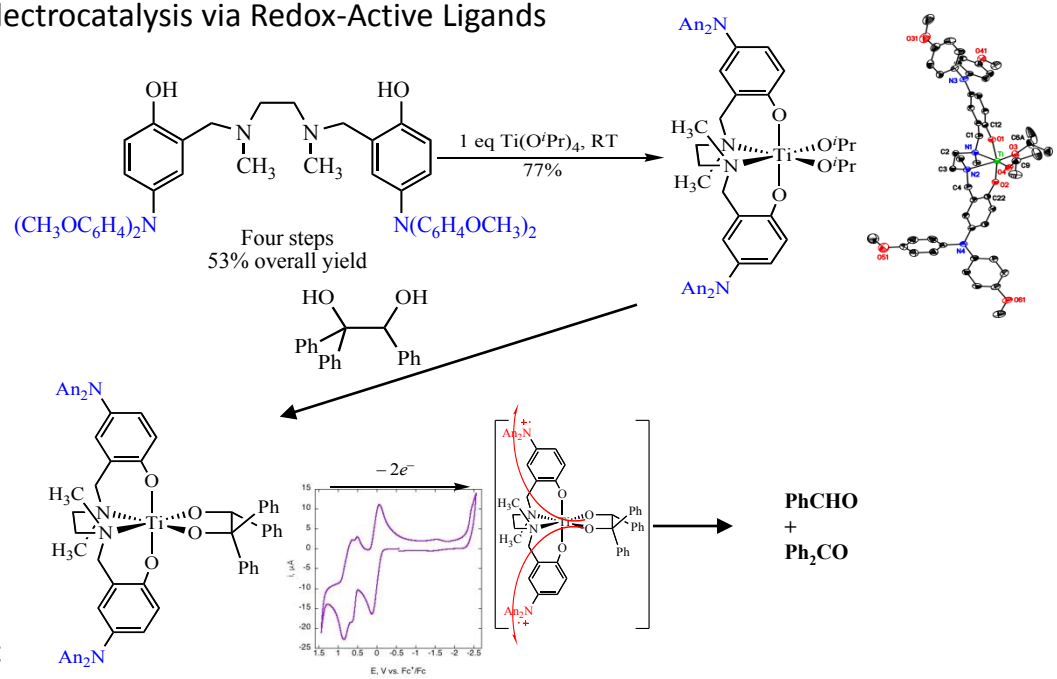
- Design and multistep synthesis of complex organic ligands
- Synthesis of soluble discrete inorganic organometallic compounds
- Characterization (NMR, IR, MS, CD, UV-Vis, X-ray, electrochemistry)
- Pedestrian electronic structure calculations

Mechanistic Study:

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

Current Energy Research

Electrocatalysis via Redox-Active Ligands



Potential SEI Research

Dioxygen Activation/Production

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

Carbon Dioxide Activation by Novel Mechanisms

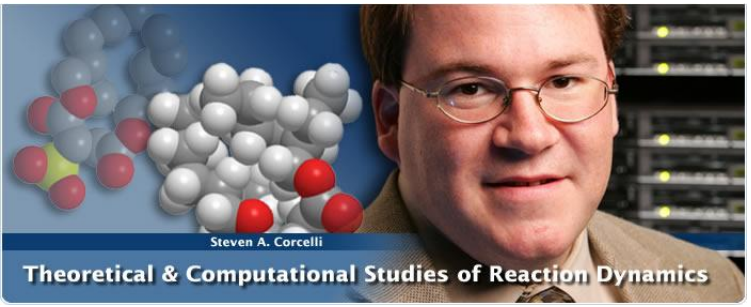
- Hydride transfer from redox-active ligands/metal hydroxides?
- Organoelectrocatalysis?

Technologies Enabled by Highly Chemoselective Electrocatalysts (collaborators?)

- Membraneless fuel cells?
- Direct solar-to-chemical fuel transformation based on (asymmetric) semiconductor nanoparticles?

Steven Corcelli

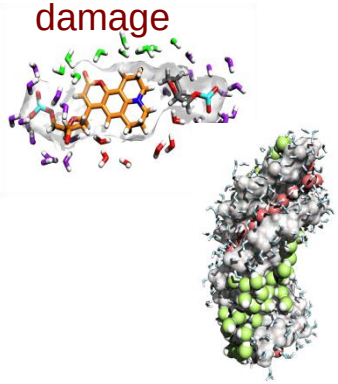
- Assistant Professor of Chemistry and Biochemistry



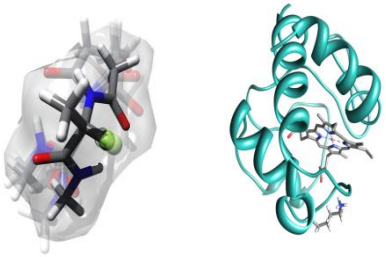
Capabilities

- 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

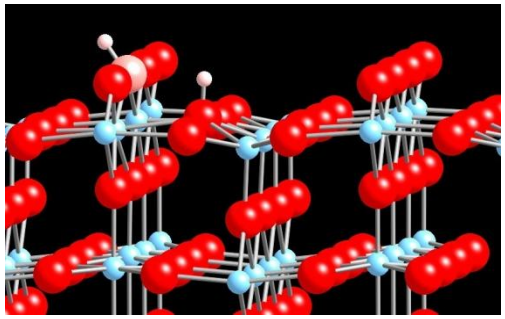
DNA hydration and damage



Infrared probes of biomolecular dynamics

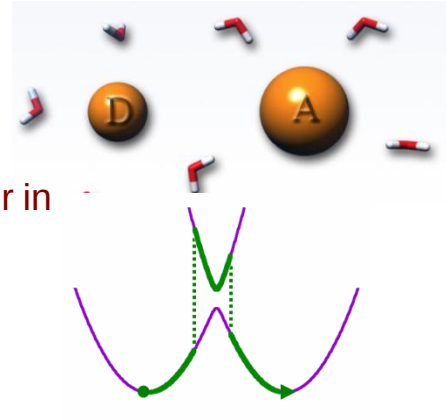


Current Energy Research



Computer simulations of aqueous metal oxide interfaces

Collaboration with Bill Schneider and Kathie Newman



Nonadiabatic charge transfer in the condensed-phase

Potential SEI 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
- Molecular dynamics simulations of photocatalysis
- Novel vibrational probes of ultrafast charge transfer

Bruce Bunker

•Professor of Physics

Capabilities

Structural characterization of nanosystems
- •TEM
  - • Lattice imaging
  - • electron diffraction
- •Scanning probe microscopy
  - • AFM/STM/MFM
- •Optical measurements
  - • Surface plasmon resonance for nanoparticles
- •X-ray techniques
  - • Diffraction, diffuse scattering, XAFS

Current Energy Research

- *In-situ* measurements of ZnO nanowire growth to determine competing growth mechanisms
- Time-dependent structure and interdiffusion in core-shell nanoparticles
- *In-situ* studies of nanoparticle-catalyzed growth of nanowires
- Bacterial biomineralization and dissolution at mineral surfaces
- Environmental nanoparticles (e.g. hematite, goethite, others)

Potential SEI Research

Luis Fernández-Torres

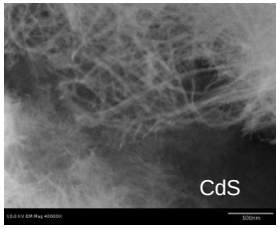
PICTURE HERE

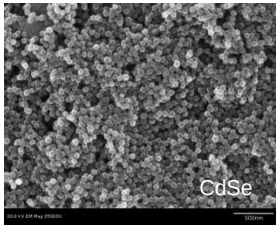
- Research Assistant Professor of Chemistry and Biochemistry
- NDnano

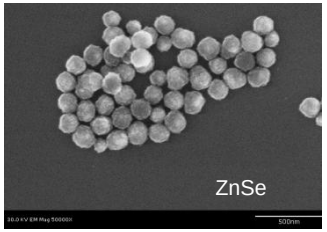
Current Energy Research

Synthesis of novel nanostructures of transition metal chalchogenides

- 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







Capabilities

Surface Science

- Experimental techniques like XPS, STM, AFM, IRRAS, Temperature Programmed Desorption (TPD)

Tribology

- Frictional properties determined by chemical interactions and reactions

Materials Chemistry

- Synthesis of novel nanostructures of transition metals and transition metal chalchogenides

Potential SEI Research

Transformative Solar Thrust

- NSF CHE Synthesis and controlled assembly of semiconductor nanostructures – submitted 11/27/09 $201,460 (still pending)

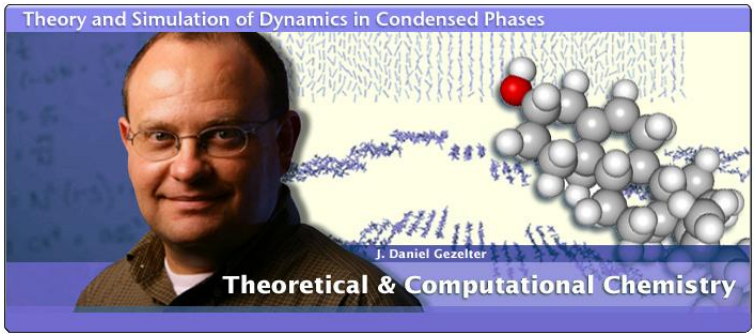
Cleaner Fossil Fuel Processes Thrust *

- 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 heteregeneous catalysts – use of buffer-layer assisted growth of metal nanoparticles on metal-oxide supports
- Novel synthesis and tribological characterization of layered transition metal chalchogenides – thin films or lubricant formulation additives of MoS2, MoSe2, WS2, WSe2, and VS2, VSe2 nanostructures

*Since 1980, reducing friction in automotive components has lead 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)

J. Daniel Gezelter

- Associate Professor o Chemistry and Biochemistry
- Director of Graduate Admissions



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

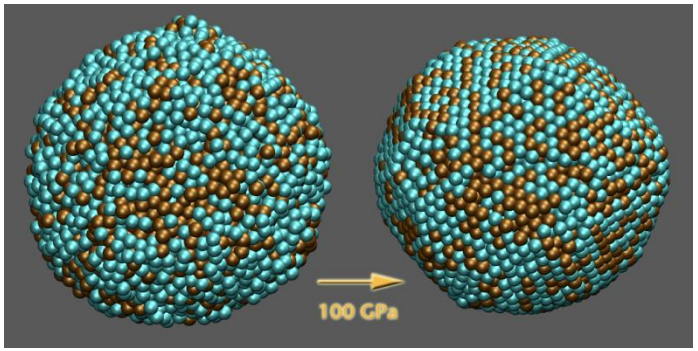
Water & Ice:
- Thermodynamics of insect anti-freeze protein (AFP) binding to ice
- Novel ice polymorphs
- Ion migration in thermal gradients

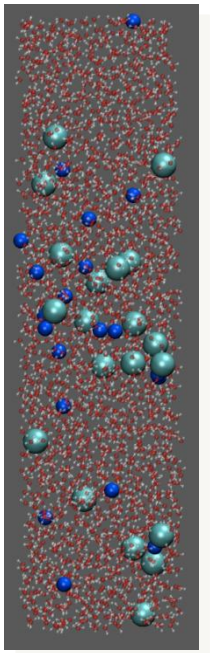
Metals & Nanoparticles:
- Models for metal–capping agent and metal–water interactions
- Particle-to-solvent thermal transport
- Alloying and de-alloying in bimetallics

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]



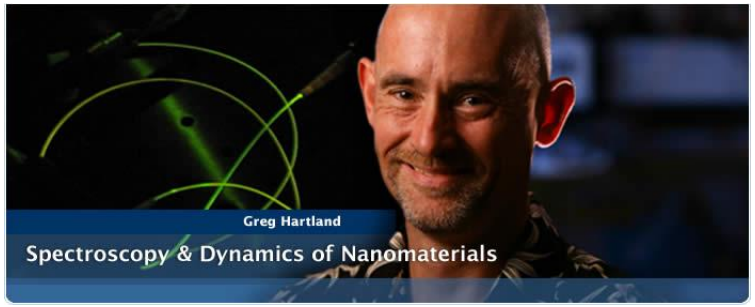


Potential SEI Research

- 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 H_2O reactors]
- Reactive bond-order force fields [chemistry]

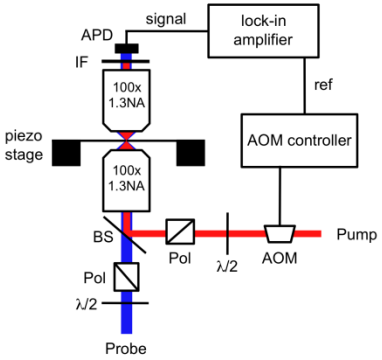
Gregory Hartland

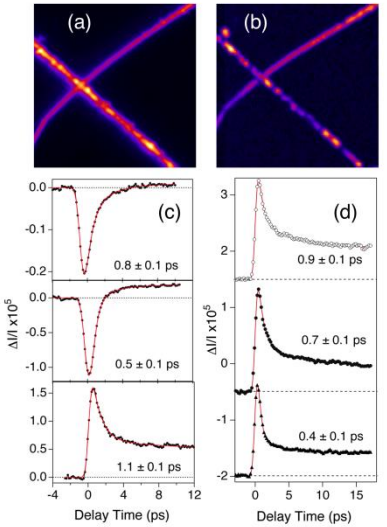
- Professor of Chemistry and Biochemistry



Current Research

Transient absorption spectroscopy of single semiconductor nanostructures





different CdTe nanowires

same wire different positions

Capabilities

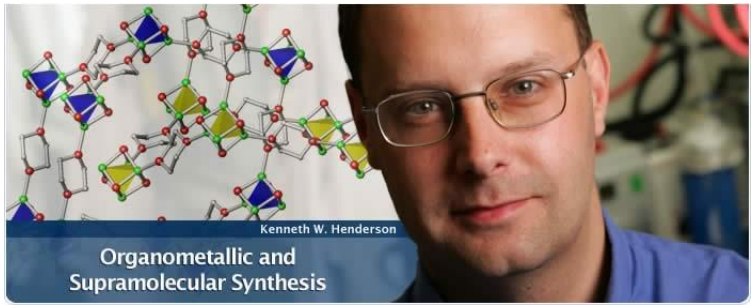
Using optics to examine the properties of nanomaterials. Current emphasis is on single particle experiments, both steady state spectroscopy studies and time-resolved measurements. Some specific topics of interest are:

- Effect of size, shape and composition on the properties of nanomaterials.
- Development and application of novel optical imaging techniques.
- Energy and charge flow in nanostructures.

Potential SEI Research

Kenneth Henderson

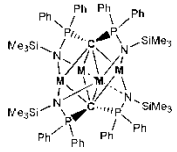
- Professor and Department Chair of Chemistry and Biochemistry
- Associate Director, Sustainable Energy Initiative

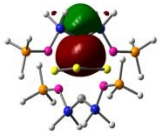


Capabilities

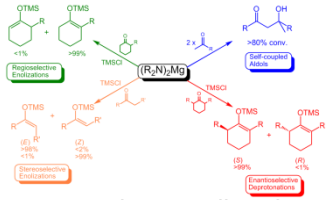
Inorganic synthesis and characterization
Organometallic s-block chemistry
- (Li—Cs, Mg—Ba)
- organic methodology development

Metal-organic frameworks
Solution structure and dynamics
Solid-state structure
Basic user of theory (DFT)

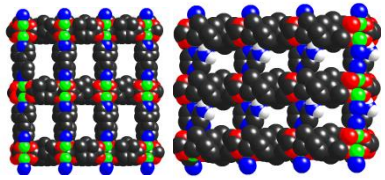




Geminal Dianions: R_2CM_2 M=Li, Na, K



Magnesium-mediated synthesis

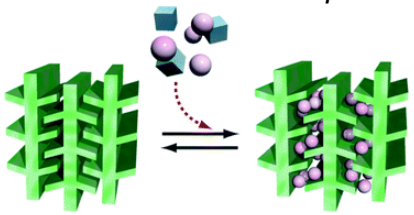


Metal-organic frameworks

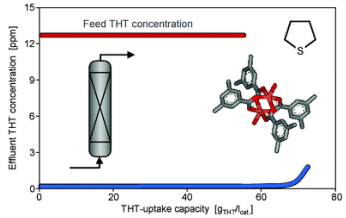
Current Energy Research

Metal-Organic Framework Applications

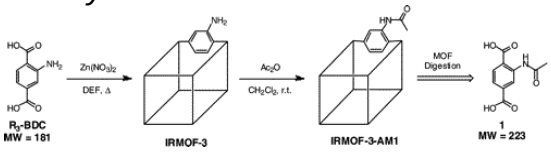
Selective Guest Uptake:



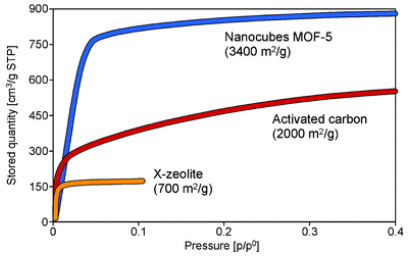
Gas Purification:



Postsynthetic Covalent Modification:



Gas Sorption:



Catalysis, membranes, nanoreactors…..

Potential SEI Research

- MOFs for CO_2 sequestration or gas purification – measurements
- Supported catalysis on high surface area materials – catalysis / measurement

Jason Hicks

•Associate Professor of Chemical and Biomolecular Engineering

Current Energy Research

- Materials for CO_2 capture from flue gas streams
- Catalytic reduction of biofuel oxygen content for use in current transportation infrastructure
- Advanced biofuels from cellulosic degradation products
- Catalyst development for biofuels production from lignin

Capabilities

- Synthesis, characterization, and application of organic / inorganic hybrid materials
- Design of high-capacity aminosilica materials for CO_2 capture from flue gas streams
- Design of well-defined aminosilica materials for mechanistic/optimization studies
- Design and development of deoxygenation catalysts for biofuels production from lignocellulosic biomass
- Upgrading of lignin to useful products

Potential SEI Research

Cleaner Fossil: Materials for gas separations

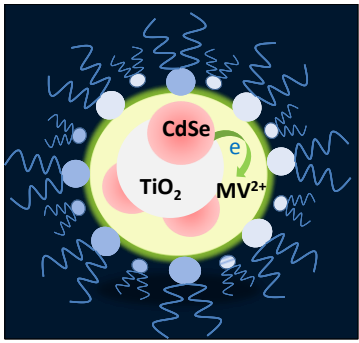
- Synthesis of amine-based organic / inorganic hybrid materials for CO_2 capture
- Synthesis of silica-tethered task specific ionic liquids for CO_2 capture

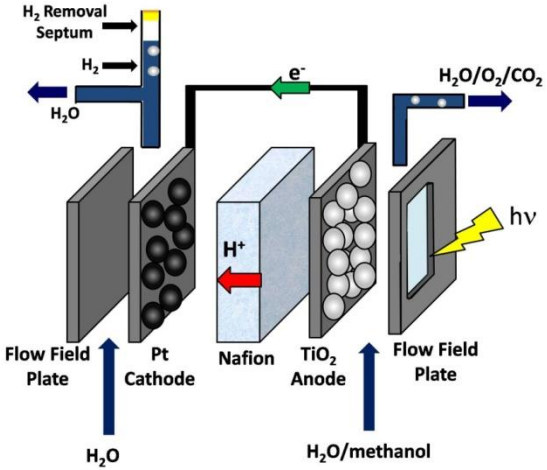
Prashant Kamat

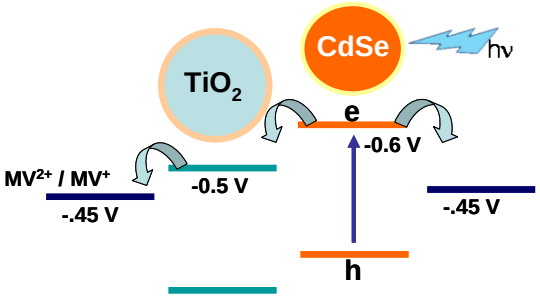
- John A. Zahm Professor of Science in Chemistry & Biochemistry
- Concurrent Professor, Department of Chemical & Biomolecular Engineering
- Radiation Laboratory
- Deputy Editor, Journal of Physical Chemistry Letters

Current Research

Solar Hydrogen production
Mapping the electron transfer processes
Improving photoconversion efficiencies





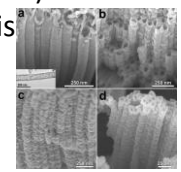


Capabilities

- Nanoparticles and Advanced Materials
  - Synthesis, characterization, and surface functionalization
  - Optical properties, Photoelectrochemistry and Sensor applications
  - Carbon nanostructures and metal nanoparticles for the developement of next generation solar cells and semiconductor metal composites for photocatalytic hydrogen production
  - Light Energy Conversion. Design of inorganic-organic nanoassemblies for light energy conversion.
- Chemical Processes in Heterogeneous Media
  - Surface photochemical processes, molecular clusters, ultrafast photophysical and photochemical events in oxides and polymers, mechanism and kinetics of photoeffects at semiconductor/electrolyte interface.
- Environmental Science
  - Advanced oxidation processes for treating organic wastes from water - use of metal oxide semiconductors such as TiO_2, SnO2 and ZnO to sense and degrade haloaromatics and azo dyes. Simultaneous sensing and destruction of low level toxic organics.

Potential SEI Research

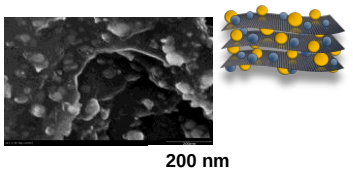
Catalyst Design
- Synthesis of new photocatalyst materials, architectures and composites
- Carbon nanostructures (CNT and graphene as catalyst suports)
- Utilization of catalysts in photoreactors and product analysis



Understanding Interfaces
- Surface science studies (XPS, EXAFS)
- Theoretical modeling & computational studies

Homogeneous catalysis (collaborative efforts in synthesis)

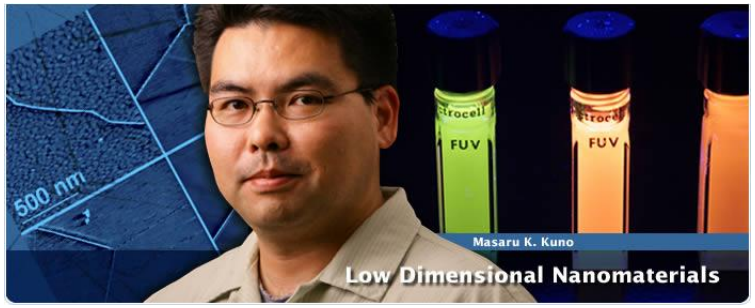
We can undertake:
- Electrochemical characterization/reduction
- Anchor on oxides
- Excited state interactions
- Product analysis



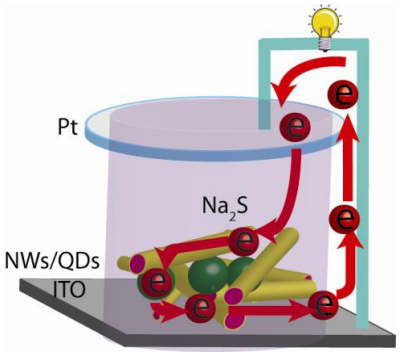
Target photoinduced H_2 production, CO_2 Reduction, Reforming hydrocarbons

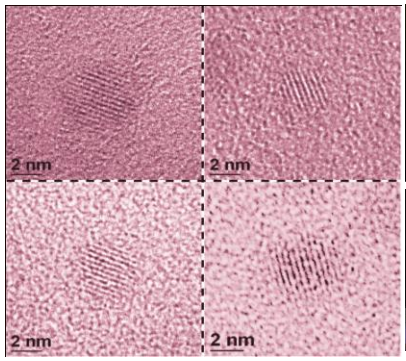
Masaru (Ken) Kuno

•Associate Professor of Chemistry and Biochemistry



Current Research

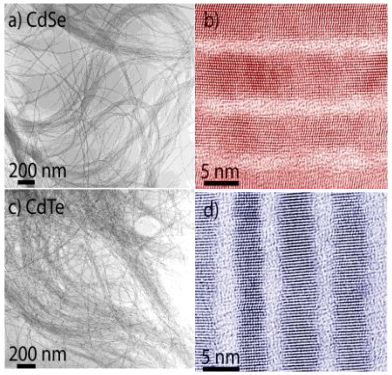


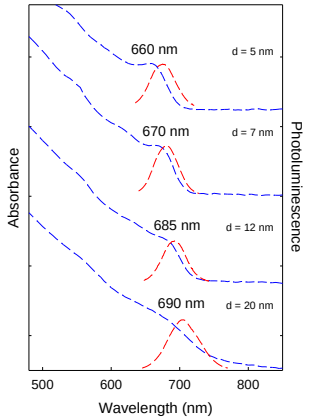


- Quantum dot (photoelectrochemical) solar cells
- Nanowire (photoelectrochemical) solar cells
- Solid state photovoltaics
- **Summary: Solar to electricity , photovoltaics**.

Capabilities

Synthetic capability and optical capability





- Synthesis of nanowires
- Synthesis of quantum dots
- Optical properties of both at the ensemble and single level

Potential SEI Research

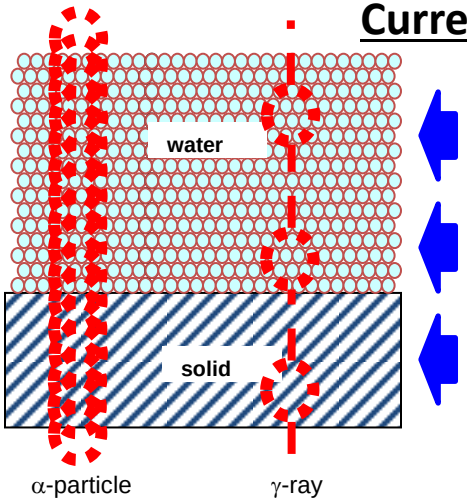
Transformative Solar: materials for the efficient conversion of solar to chemical energy – the creation of transformative solar cell technologies.

- Look into the synthesis and characterization of metal oxide nanostructures. (water splitting purposes, for example)
- Collaboration for selection of systems to investigate, given that my focus has been on (relatively speaking) low gap semiconductors.
- Optical characterization of these materials and potential devices.

Jay LaVerne

- Professional Specialist, Radiation Laboratory
- Research Professor, Physics

Current Research



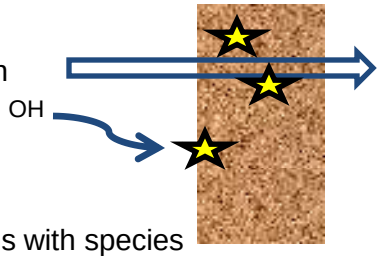
Safer Storage of Materials

- What effects occur in the bulk water?
- What happen at the interface?
- How do processes in the solid affect the interface or water?

Actinide Materials Stabilization

Self radiolysis will modify virtually all actinide systems

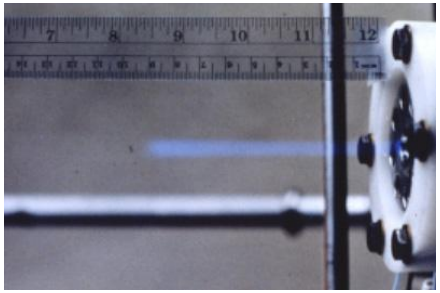
changes to chemical composition
modifications to physical state
decrease in stability
loss of functionality



Indirect damage by reactions with species produced by radiolysis of the environment
Direct damage by energy deposition in material

Capabilities

physics → chemistry → materials / engineering / environment



- Examine energy loss, charge and other properties of ionizing radiation
- Elucidate fundamental radiolytic decomposition of molecules and the kinetics of the transients

Potential SEI Research

- Experimental examination of irradiated surfaces theoretical characterization of surface species
- May be possible to irradiate actinide materials to accelerate radiation ageing processes using specific types of radiation

Safe Nuclear → actinide materials stabilization → safer storage of materials

Edward Maginn

- Professor of Chemical and Biomolecular Engineering
- Graduate School Associate Dean of Academic Programs

Current Energy Research

Ionic liquids

- CO_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

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 *ab initio* simulations

Systems of interest

- Liquids, crystalline materials, nanoporous materials

Potential SEI 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 (Cleaner fossil, safer nuclear)

- H_2/CO_2 separation
  - sorption and diffusion in nanoporous materials (MOFS, membranes)
- Ionic conductivity in Ils
  - Mechanism of conduction
- Behavior of confined ILs in separation applications (SILMs)
  - PFG NMR, single-molecule probes of ILs confined in nanopores
  - Bulk sorption behavior
- Ion exchange materials
  - Selectivity, rates (actinide separation / storage)

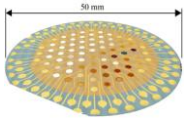
Paul McGinn

- Professor of Chemical and Biomolecular Engineering

Capabilities

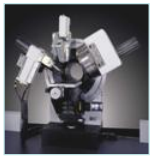
High-throughput materials development and characterization

Processing

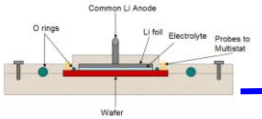


Annealed Library

Characterization



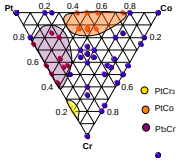
Automated XRD



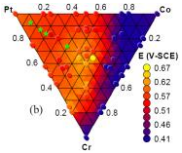
Parallel electrochemical characterization

Automated OM

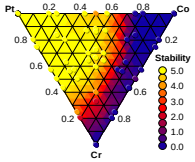
Analysis



Structure



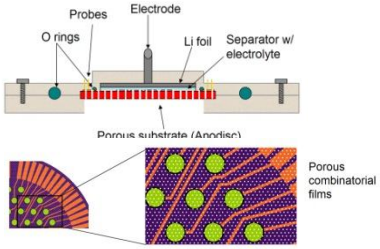
Capacity



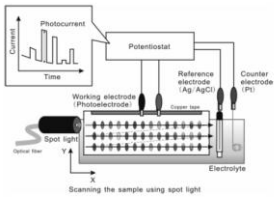
degradation

Current Energy Research

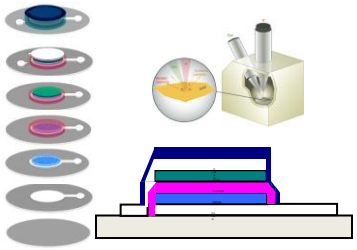
Li-Air Cathode Catalysts



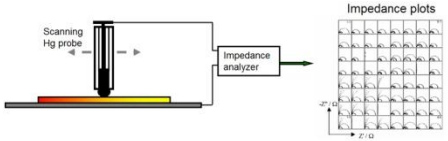
Photocatalysts for electrolysis / solar



Thin Film Battery Interfaces



Solid State Electrolytes



Potential SEI Research

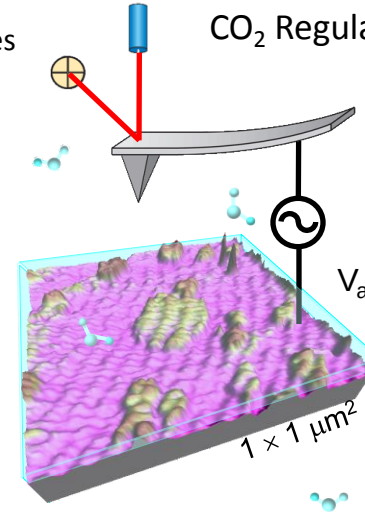
XXX

Chongzheng Na

- Assistant Professor, Civil Engineering and Geological Sciences

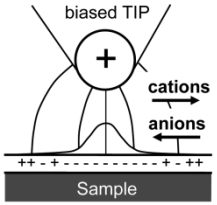
Current Research

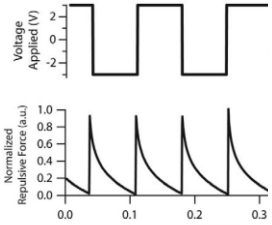
CO_2 Regulation of the Ion Mobility on Carbonate Surfaces



$$CO_2 + MeCO_3(s) + H_2O \rightleftharpoons Me^{2+}(aq) + HCO_3^-$$

Me = Ca, Mn, Fe, Mg, Zn, and etc.

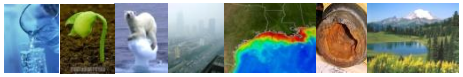




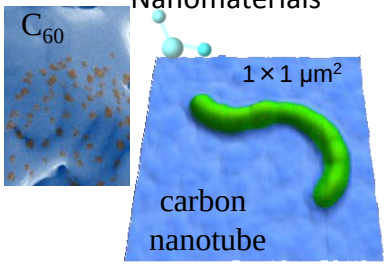
$$\Delta F(t) = Ae^{-t/\tau}$$

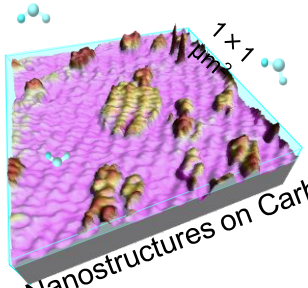
$$D = \tau^{-1}\alpha_1^{-2}\ \alpha_1 = 2.4 \times 10^8\ m^{-1}$$

Capabilities



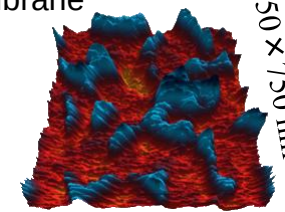
Microscopic Recognition of Molecules & Nanomaterials





Oxide Nanostructures on Carbonate

Lipid Rafts in Fungal Membrane

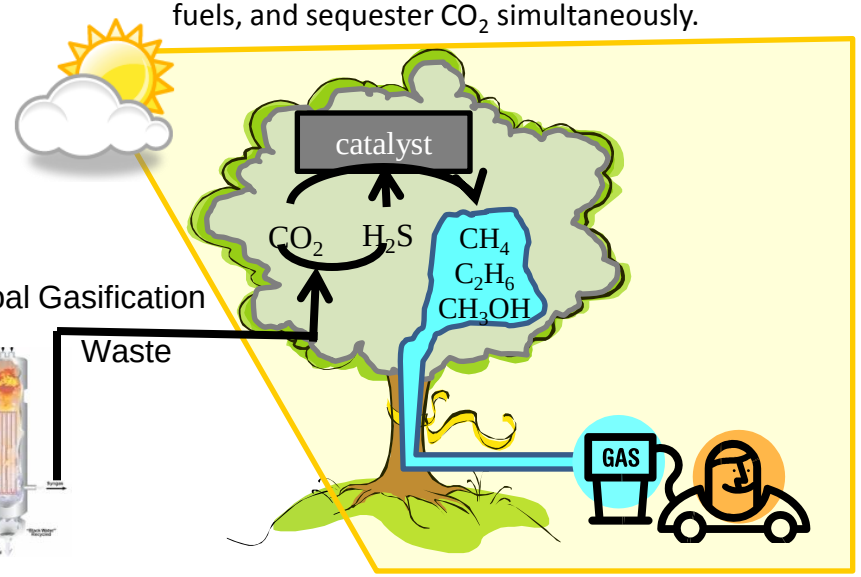


Molecular Approach for Biofilm Prevention & Stimulation in Water Treatment

Mineral-Liquid Interfacial Chemistry & Physics

Potential SEI Research

Planting "trees" to fix solar energy, produce chemical fuels, and sequester CO_2 simultaneously.



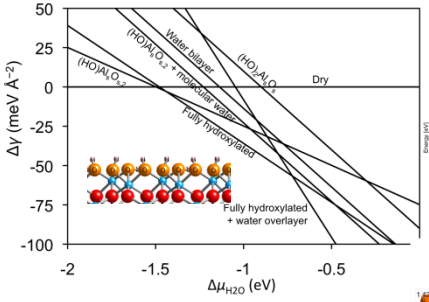
William Schneider

- Professor of Chemical and Biomolecular Engineering
- Professor of Chemistry and Biochemistry

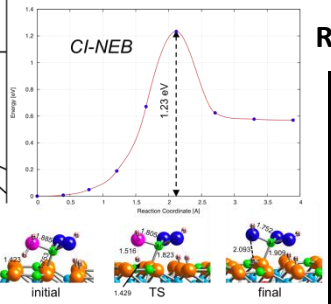
Capabilities

- 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

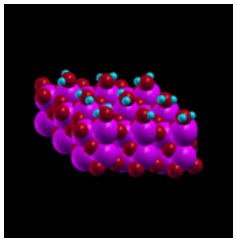
Structures & thermodynamics



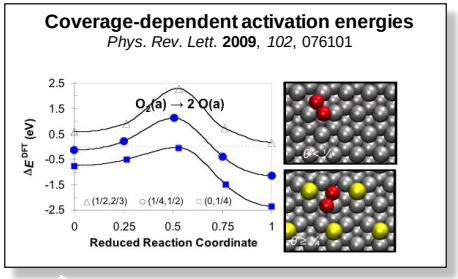
Reaction Rates

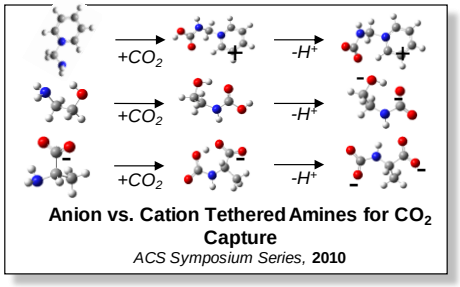


Reaction dynamics

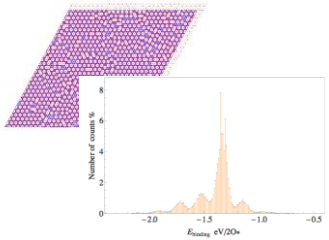


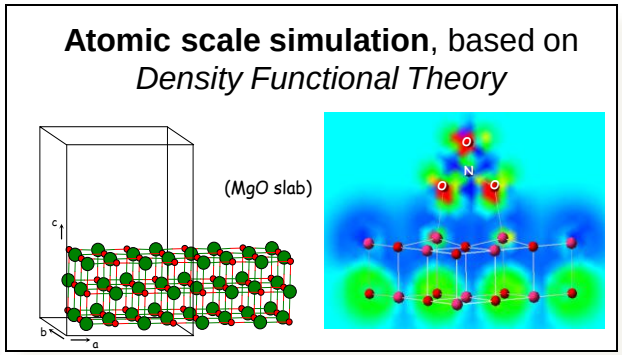
Current Research





Environmental effects on surface kinetics





Specific Areas of Research

- Ionic Liquids for CO_2 Capture
- Catalytic NO oxidation
- Water gas shift
- Catalytic NO reduction
- Perovskite catalysis

Potential SEI Research

Collaboration on site-specific/homogeneous energy-related catalysis

Mark Stadtherr

- Keating-Crawford Professor of Chemical and Biomolecular Engineering

Current Energy Research

Molecular Thermodynamic Models of Mixtures Involving Ionic Liquids

- Prediction of phase behavior and physical properties of ILs and mixtures
- Excess Gibbs energy models (activity coefficient models)
  - Liquid-liquid equilibrium (LLE) at low pressure
  - NRTL, electrolyte-NRTL, UNIQUAC, UNIFAC, etc.
  - Symmetric vs. asymmetric models
  - Extraction of organics (e.g., biofuels) from dilute aqueous solution
- Equation-of-state models
  - Gas solubilities in ILs
  - LLE at moderate/high pressure
  - Cubic EOS, Statistically associating fluid theory (SAFT)
  - Absorption refrigeration
- Parameter estimation requires reliable computing
- Computation of phase behavior requires reliable computing

Capabilities

Reliable Computing

- Modeling complex physical phenomena (macroscopic to molecular) through nonlinear algebraic equation sand ODEs (initial value problems). Especially interested when:
  - uncertainty in model parameters/initial conditions.
  - uncertainty characterized by (imprecise) probability distribution
  - identifying global minima (or maxima) within algebraic and dynamic constraints is required

Molecular Thermodynamic Models of Mixtures

- Apply molecular thermodynamics to develop models for of phase behavior and physical properties
- Excess Gibbs energy models (activity coefficient models)
- Equation-of-state models

Potential SEI Research

Thermodynamic modeling/Phase behavior calculations

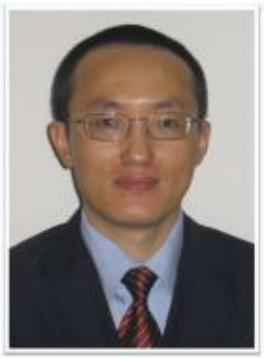
- CO_2 capture
- Gas solubilities
- Enthalpies
- Solid-fluid equilibrium
- Actinide separations

Process modeling

- Dynamics and operability
- Global sensitivities
- Safety: Regions of parameter space that result in safe operation
- Quality control: Regions of parameter space that result in on-spec product
- CO_2 capture
- Actinide separations

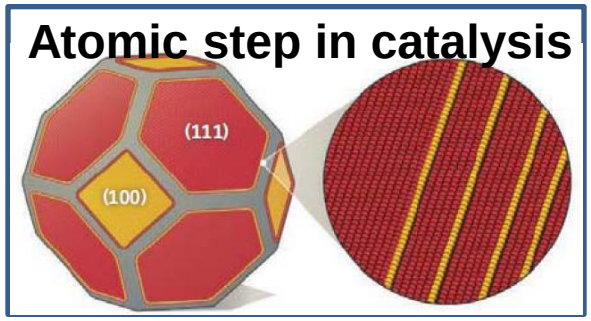
Franklin Tao

- Assistant Professor of Chemistry and Biochemistry

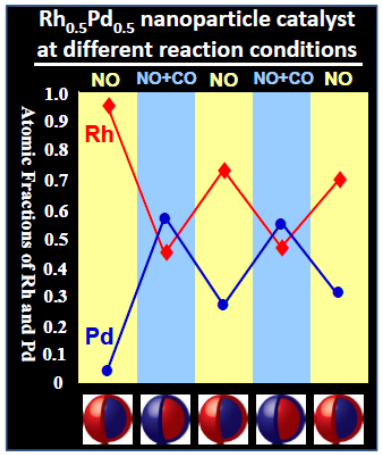


Current Energy Research

- Removal of impurity CO or NO
- Photocatalytic conversion of CO_2
- Fuel cell catalysts
- Water splitting
- Hydrocarbon conversion



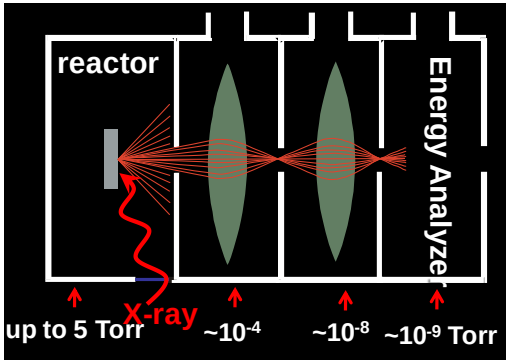
Science 327 , 789 (2010)

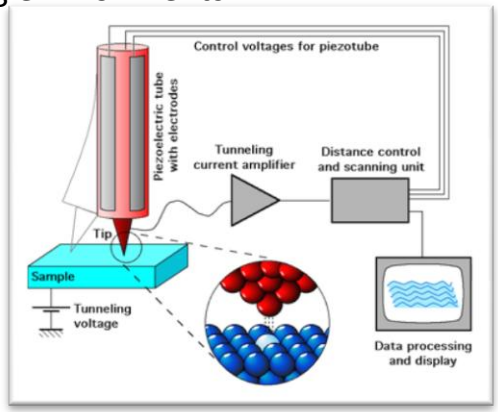


Science 322 , 932 (2008)

Capabilities

- Materials Synthesis and *In-situ* Studies of Catalysis for Efficient Energy Conversion
- High Pressure Photoelectron Spectroscopy - offers *in-situ* **chemistry** information of catalytic materials under reactions or working environments
- High Pressure Scanning Probe Microscopy - offers *in-situ* **structural** information of catalytic materials at atomic level under reactions or working environments





Potential SEI Research

Materials Synthesis and *In-situ* Studies of Catalysis for Efficient Energy Conversion

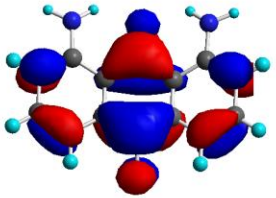
- Develop *in-situ* techniques (high pressure XPS and high pressure STM systems)
- Synthesize nanocomposite catalytic materials
- Explore *in-situ* structure and chemistry
- Build intrinsic connection between *in-situ* structure/chemistry and catalysis activity/selectivity
- Design new catalytic materials on the basis of *in-situ* studies
- Build collaborations to deal with challenges in energy conversion

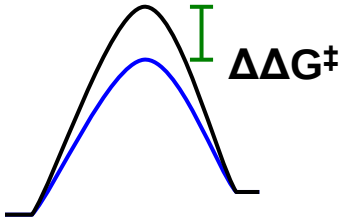
Olaf Wiest

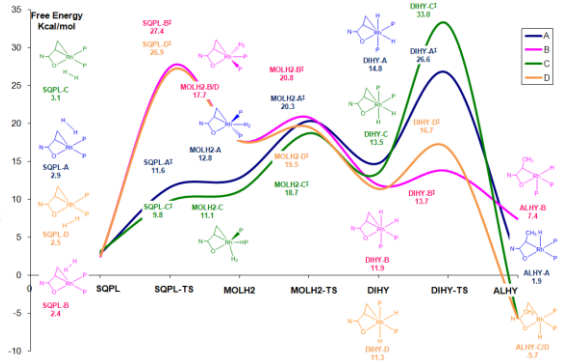
- Professor of Chemistry and Biochemistry

Current Energy Research

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

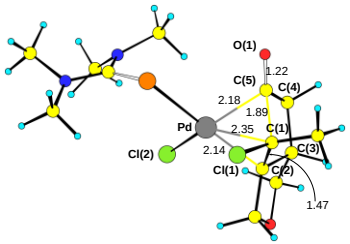


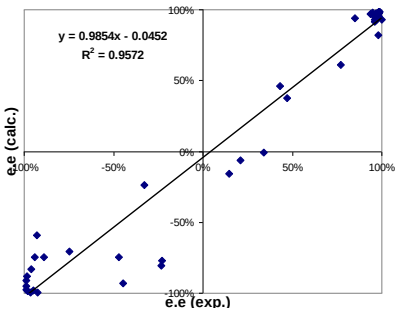




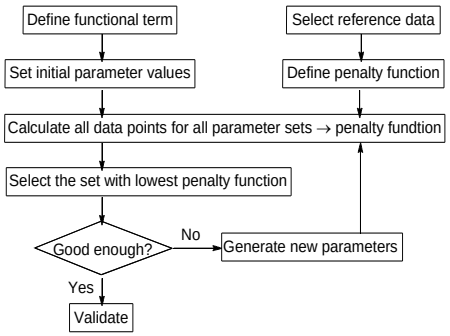
Capabilities

- 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





$$x^2 = \sum_i w_i^2 (y_i - y_i)^2$$



Potential SEI Research

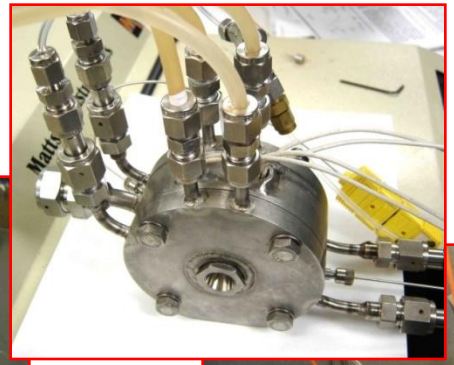
- General Computational Support
  - Geometric & electronic structures
  - Properties of small molecules
  - Force field generation
- Clean Fuel Initiatives
  - Reaction pathways & intermediates
  - Catalyst design
- Solar Energy Conversion
  - Molecular design of devices
  - Possibly synthesis of building blocks

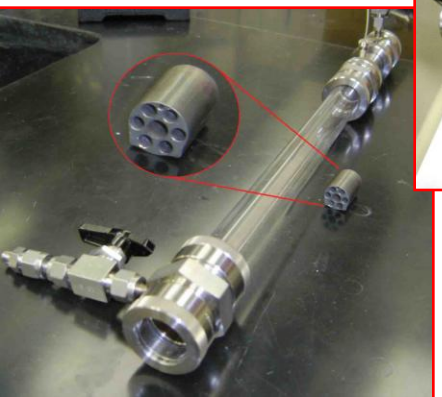
Eduardo Wolff

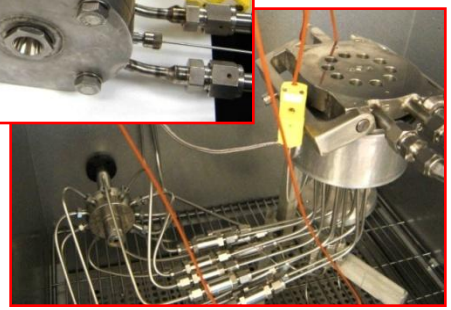
- Professor of Chemical and Biomolecular Engineering

Capabilities

- High throughput synthesis and preparation
- Prallel activity evaluation and parallel operando spectroscopy
- Kinetics simulation







Current Research

- Catalysis
- Novel Impregnated Layer Combustion Synthesis (ILCS) with Alex Mukasyan (NSF CBET 0730190)
- Cu/ZnO/ZrO2-Pd catalyst for H_2 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 SEI Research

- Transformative Solar
  - Application of the nanodiode to reduce band gap in solar cells
  - Photocatalytic production of hydrogen from water
- Clean fossil fuels: ILCS of high area
- Fe-Co oxides for FT synthesis.