THE DEPARTMENT *of*
CHEMICAL AND BIOMOLECULAR ENGINEERING
www.chbe.umd.edu

Research Overview

Sheryl Ehrman, Keystone Professor and Chair

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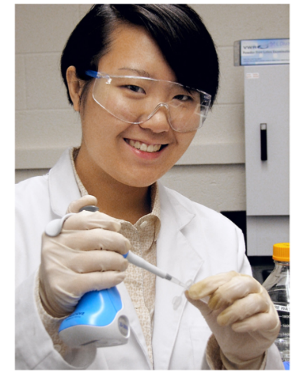
ChBE Fast Facts

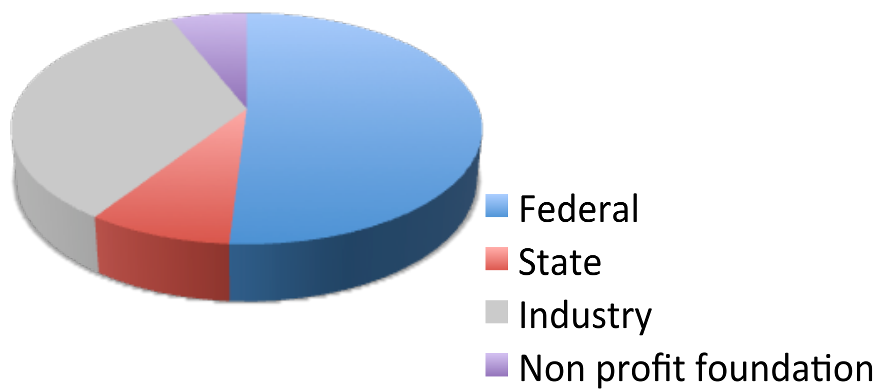


13 faculty + 1 joining January 2011

~ 320 undergraduate students

42 PhD, 14 MS students

~ 2.1 M external research expenditures FY 2010



Faculty

Raymond A. Adomaitis
Professor, Associate Chair for Graduate Studies
Systems modeling and simulation; semiconductor and thin film processing

Mikhail Anisimov
Professor
Mesoscopic and nanoscale thermodynamics, critical phenomena, and phase transitions in soft matter

Richard V. Calabrese
Professor
Multiphase flow, turbulent and mixing, computational fluid dynamics

Kyu Yong Choi
Professor, Associate Chair for Undergraduate Studies
Macromolecular and polymer reaction engineering, polymer nanomaterials

Panagiotis Dimitrakopoulos
Associate Professor
Computational fluid dynamics, bio/micro-fluidics, biophysics and numerical analysis

Sheryl H. Ehrman
Keystone Professor and Chair
Aerosol and nanoparticle technology, air pollution

Faculty

Srinivasa R. Raghavan
Associate Professor
Patrick and Marguerite Sung Chair
Complex fluids, polymeric and biomolecular self-assembly, soft nanostructures

Erich Wachsman
Professor
William L. Crentz Centennial Chair in Energy Research
Electrochemistry, solid oxide fuel cell development

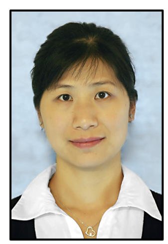
Nam Sun Wang
Associate Professor
Biochemical engineering

William A. Weigand
Professor
Biochemical engineering, bioprocess control and optimization

Jeffrey Klauda
Assistant Professor
Biophysics and thermodynamics

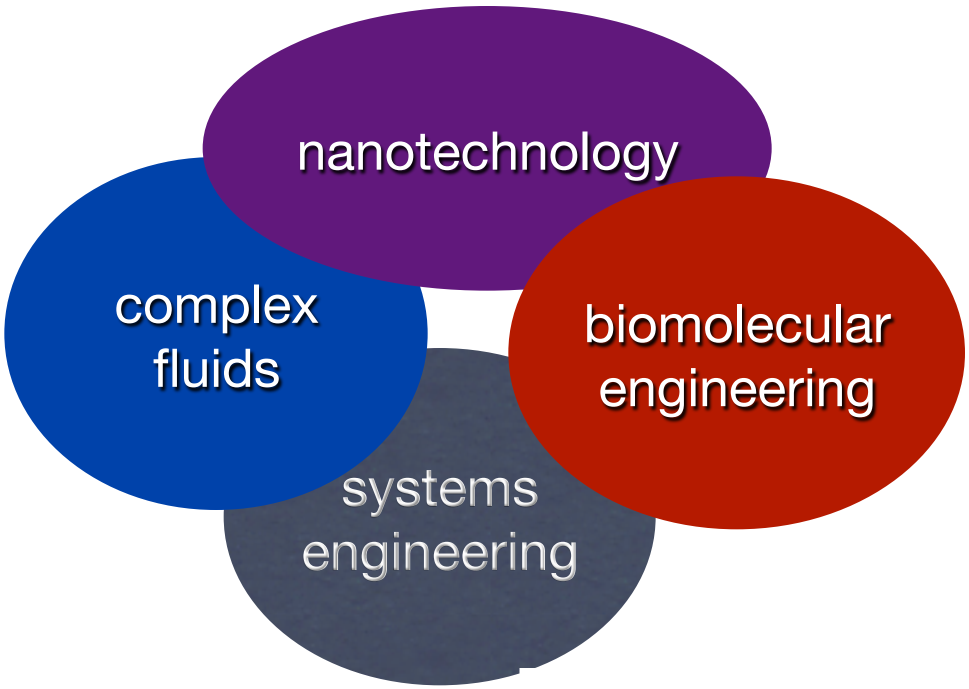
Ganesh Sriram
Assistant Professor
Systems biology and metabolic engineering

Chunsheng Wang
Assistant Professor
Energy conversion and storage



Dongxia Liu
Assistant Professor
Zeolite materials for catalysis and separations

Department Research Strengths



Engineering Strategic Research Areas:

Biotechnology
Nanotechnology
Sustainably engineered systems

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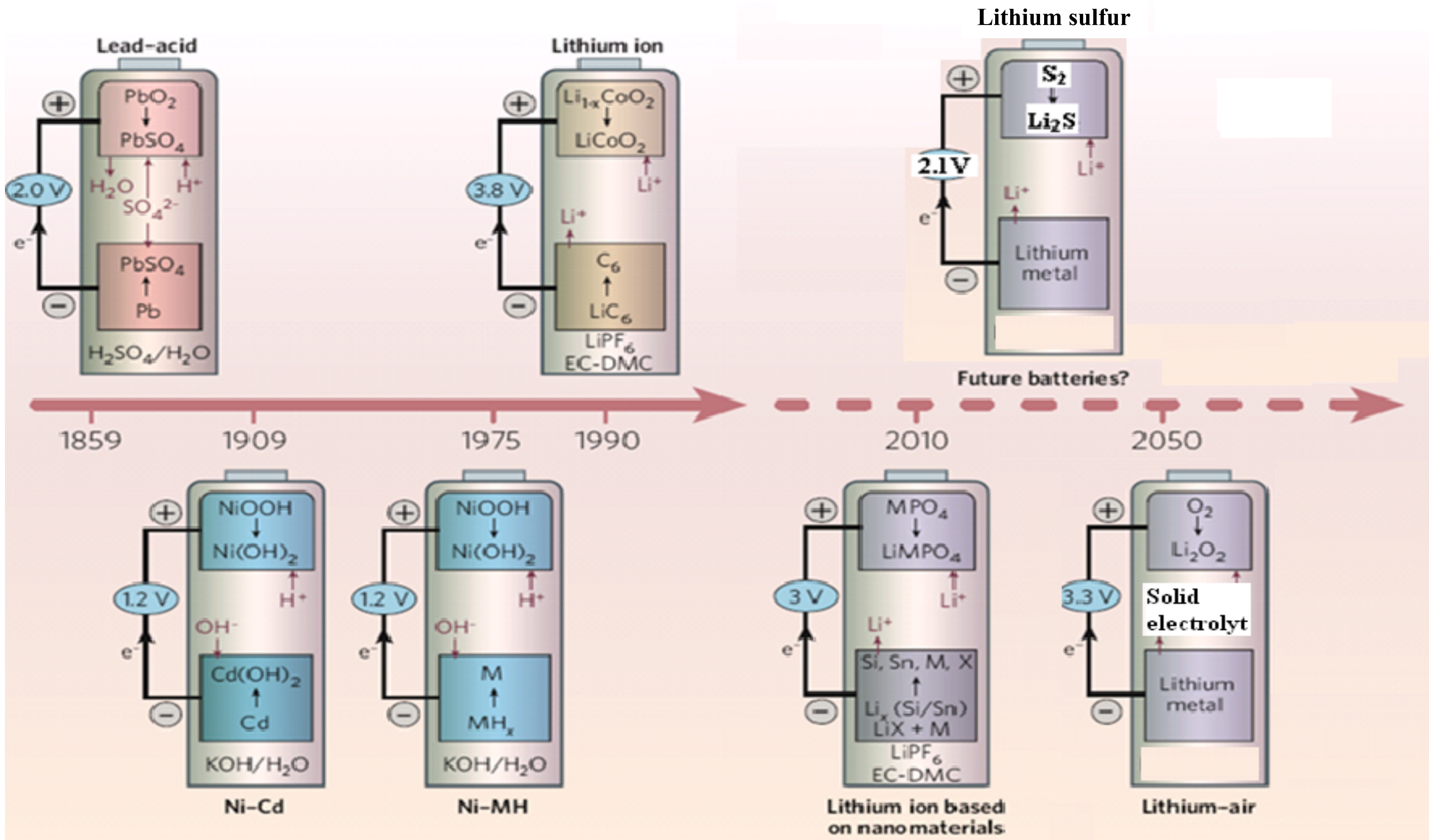
Some current research interests:

- Energy: Li-ion batteries, biofuels, solar hydrogen
- CO_2 sequestration and storage
- Nanomaterials and biological barriers

Energy Storage: Li-ion Battery Materials and Systems

Chunsheng Wang – ChBE, in collaboration with:
Kyu Yong Choi – ChBE
Sheryl Ehrman – ChBE
Srini Raghavan - ChBE
Reza Ghodssi – ISR/ECE
James Culver – Plant Science and Landscape Architecture
Peter Kofinas – BIOE
Kang Xu – Army Research Laboratory, Adelphi MD

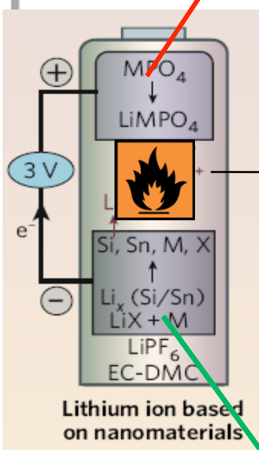
Research Battery History and Future



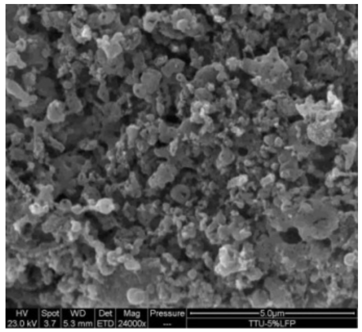
M. Armand and J. M. Tarason, Nature, 451 (2008)652

Li-ion Battery Research

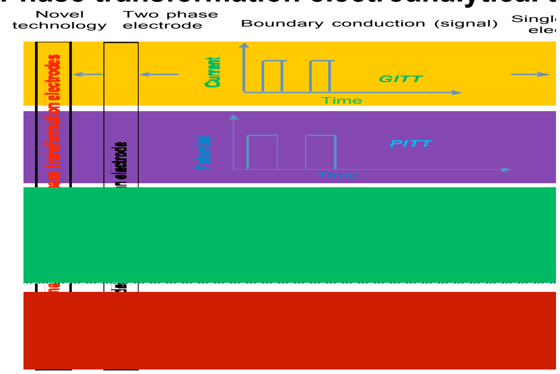
2010



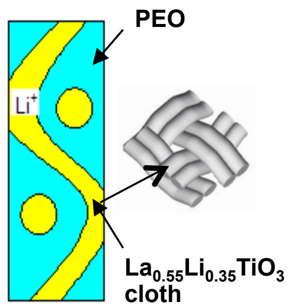
Micro-sized nanoporous $LiMPO_4$ cathodes



Phase transformation electroanalytical techniques

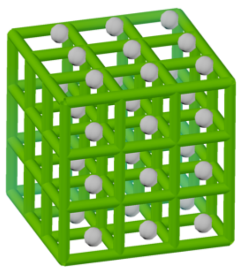


Dry solid electrolytes

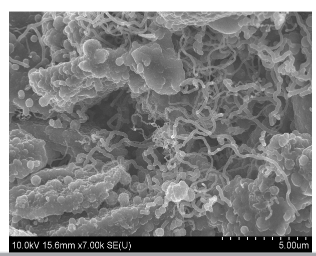


Flexible LLTO –PEO electrolyte

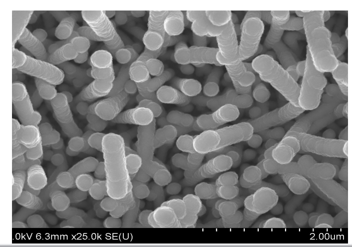
Scaffold Si Anodes



CNT coated Si anodes



Virus-Enabled Silicon Anodes



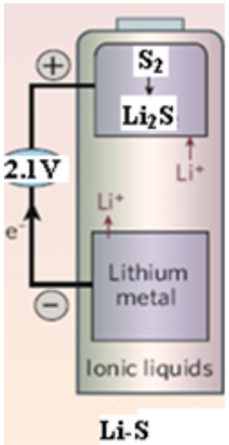
Achievements

1. *Journal of Physical Chemistry C,* 114(2010)2830
2. *Journal of Power Sources, 196 (2010)1442*
3. *Journal of Electrochemical Society,* 152 (2005) A205
4. *Advanced Functional Materials, in press*
5. *ACS Nano, 4*(2010)5366
6. *Chemistry Communications,* 46 (2010)1428
7. *Journal of Materials Chemistry,* 20(2010)5035
8. *Electrochemistry Communications,*12(2010)98

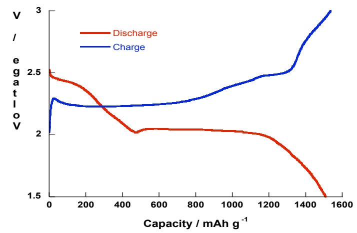
Research on Next Generation Li-ion Batteries

2010

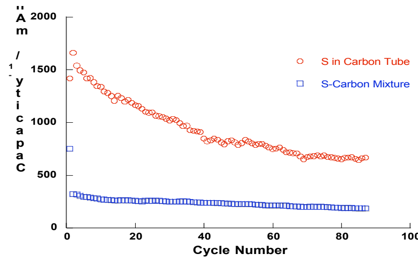
2050



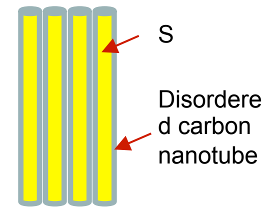
Li-S

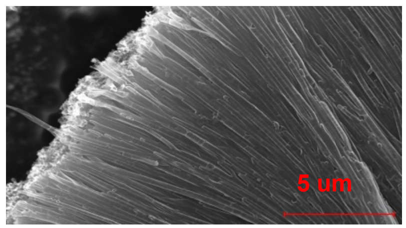


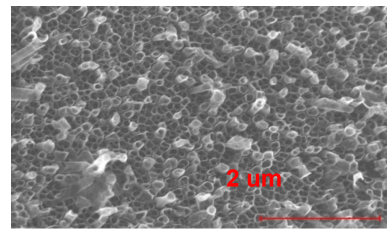
Discharge/Charge Curves



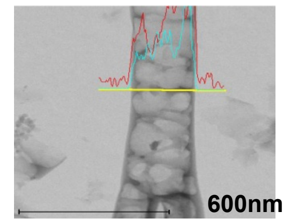
Cyclability



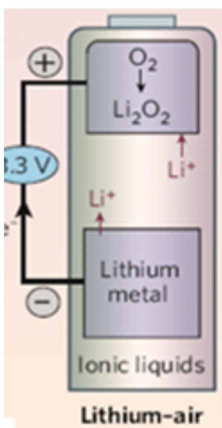




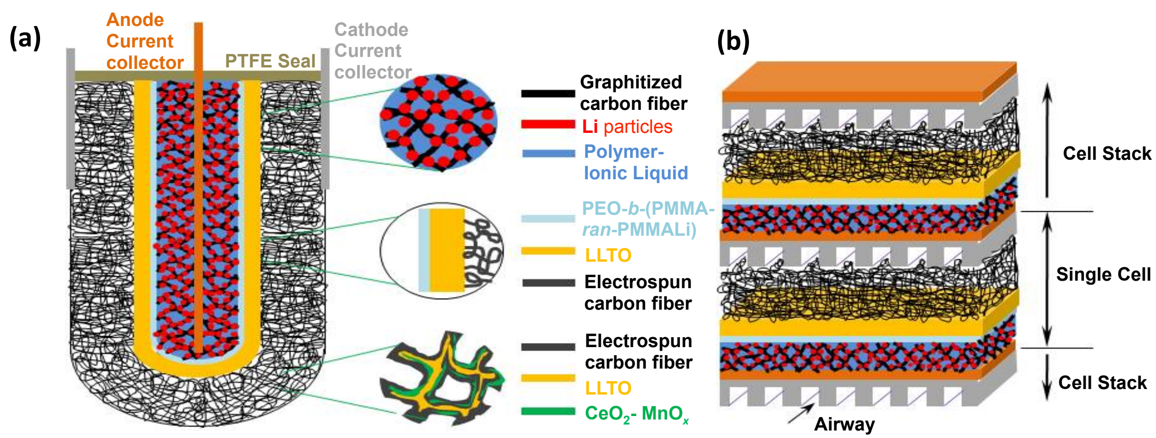
SEM images



S and C EDX Analysis



Lithium-air

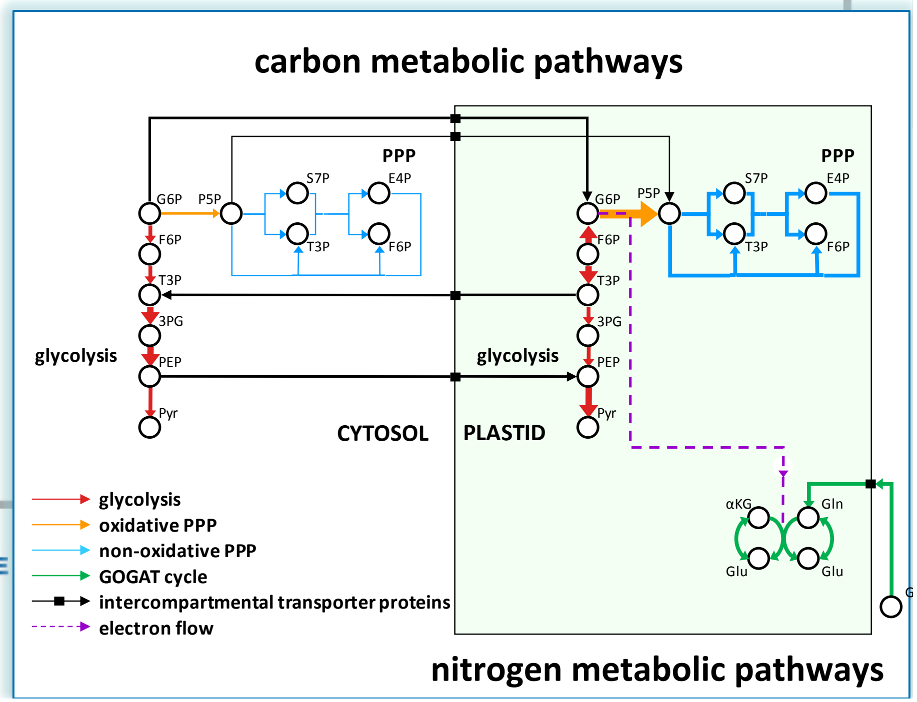


Schematic of (a) the proposed tubular Li-air cell, (b) the proposed planar Li-air cells in stack.

Energy: Using systems biology to investigate nitrogen efficiency in a bioenergy feedstock

- Overarching objective: Engineering trees with improved nitrogen use efficiency and biomass productivity
- Poplar is a future bioenergy feedstock
  - Does not require farmland, does not conflict with food supply
  - Nitrogen crucially determines productivity
  - Quantification of metabolic and regulatory networks
- Collaboration with Ganesh Sriram, ChBE and Professor Gary Coleman (Plant Sciences, University of Maryland), expert in poplar molecular biology
- Funded by NSF Plant Genome Project award

Picture from article in The Baltimore Sun



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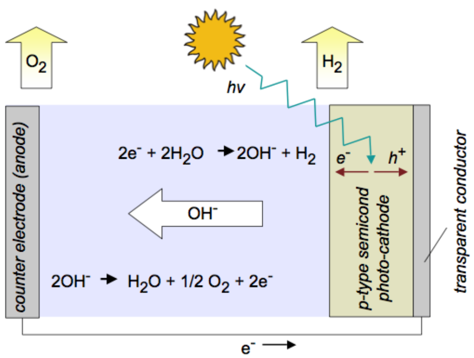
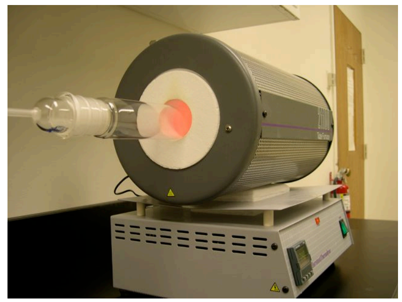
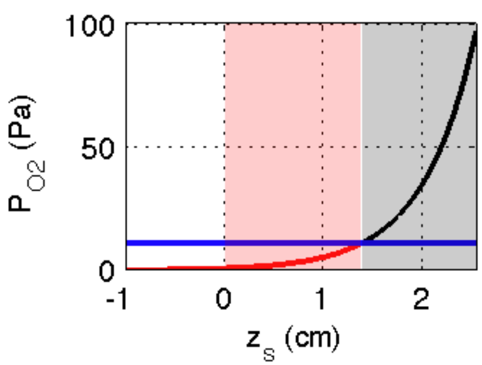
THE

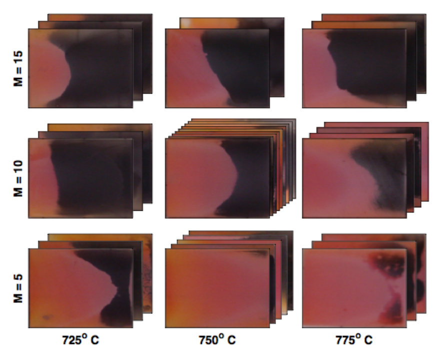
Energy: Solar Hydrogen Generation

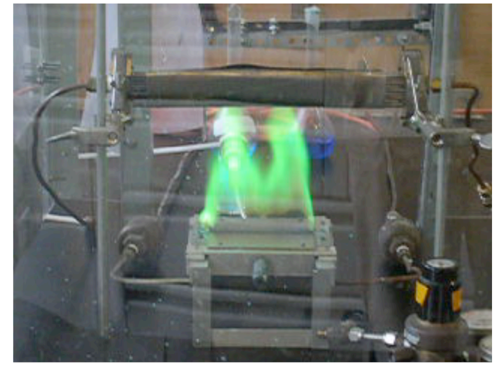
Modeling and experimental development of earth abundant semiconductor materials for solar splitting of water to produce hydrogen and oxygen.
Adomaitis, Ehrman, ChBE, Zachariah (ME/CHEM)

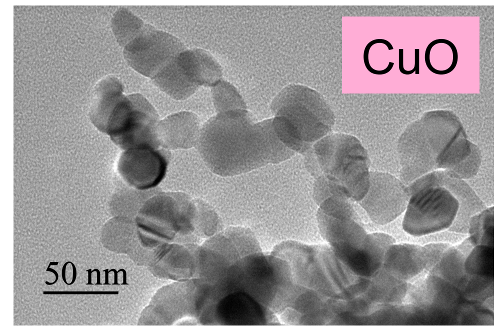


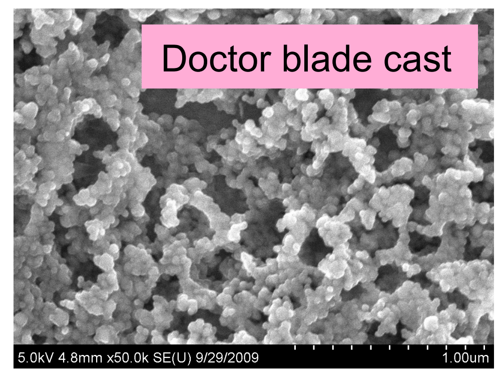












CO_2 Sequestration and Storage

Richard V. Calabrese, ChBE
- Prediction (CFD) & measurement of turbulent velocity fields
- Particle-fluid & gas/liquid-liquid dispersion
- Modeling of particle scale transport phenomena

Kyu Yong Choi, ChBE
- Polymer Reaction Engineering
- Design and development of polymer substrates

Jeffrey B. Klauda, ChBE
- Multi-scale modeling & molecular simulation
- Gas hydrates

Others: Adomaitis, Dimitrakopoulos, Ehrman

Development of Novel Carbon Capture Technologies Requires a Continuum of Effort Across Multiple Length Scales

Pre-combustion capture

Post-combustion capture

Solid sorbents and liquid solvents

Membranes

Solvent impregnated substrates

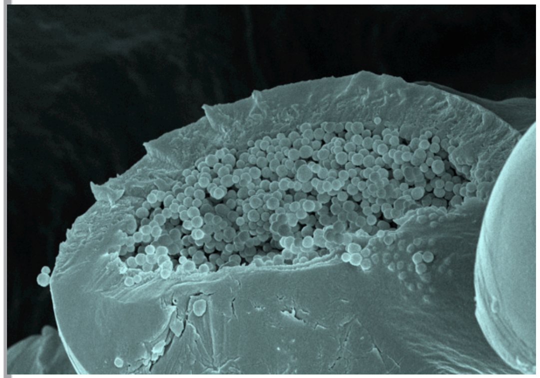
Molecular Scale	Particle Scale	Device Scale	Plant Scale
Materials discovery	Engineered particles & membranes	Design of fixed/ fluidized beds, packed/tray towers & membrane trains	Process integration
Materials characterization	Single particle behavior – thermodynamics; transport & reaction rates	Pilot scale design & demonstration	Plant scale design & demonstration
Molecular simulation/ computational screening	Particle scale rate models	CFD modeling	Process simulation

Functionalized Ultra-Porous Silica as a Novel Absorbent for CO_2 Capture

K. Y. Choi, Professor
Polymer Reaction Engineering Laboratory
Department of Chemical & Biomolecular Engineering
University of Maryland

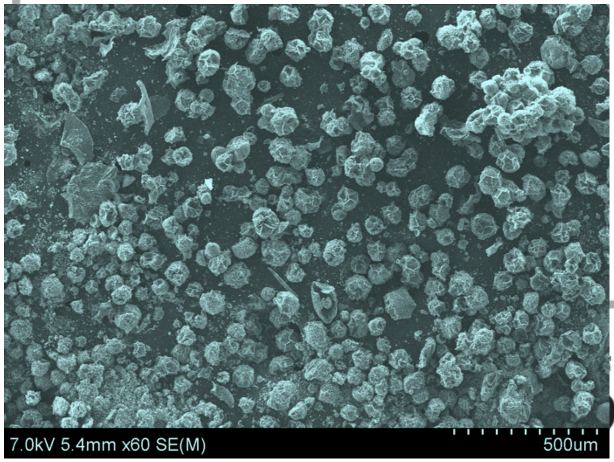
Synthesis of Inverse Opal-Like 3D-Particle Structure

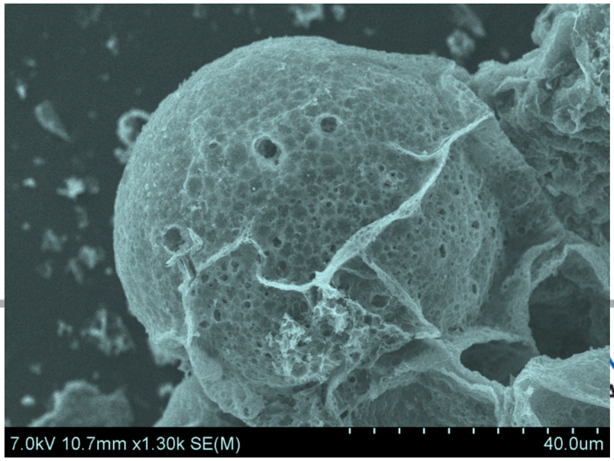
Formation of micron-sized polymer particles with controlled internal structures that encapsulate inorganic precursors (sacrificial template).

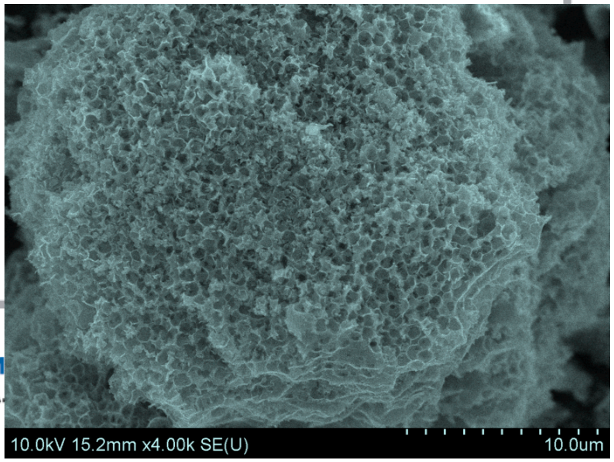


Core-shell pomegranate-like structures
synthesized by Micro-dispersive polymerization in confined reaction space (MDPCRS)

Catalytic reaction of the inorganic precursor and selective removal of the polymeric template.





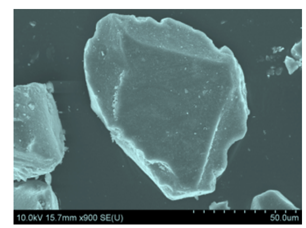
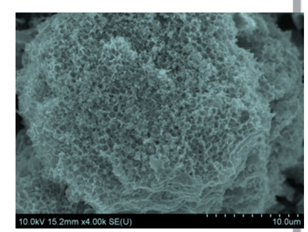


Ultra-Porous Inverse Opal-Like Silica (UP-IOS)

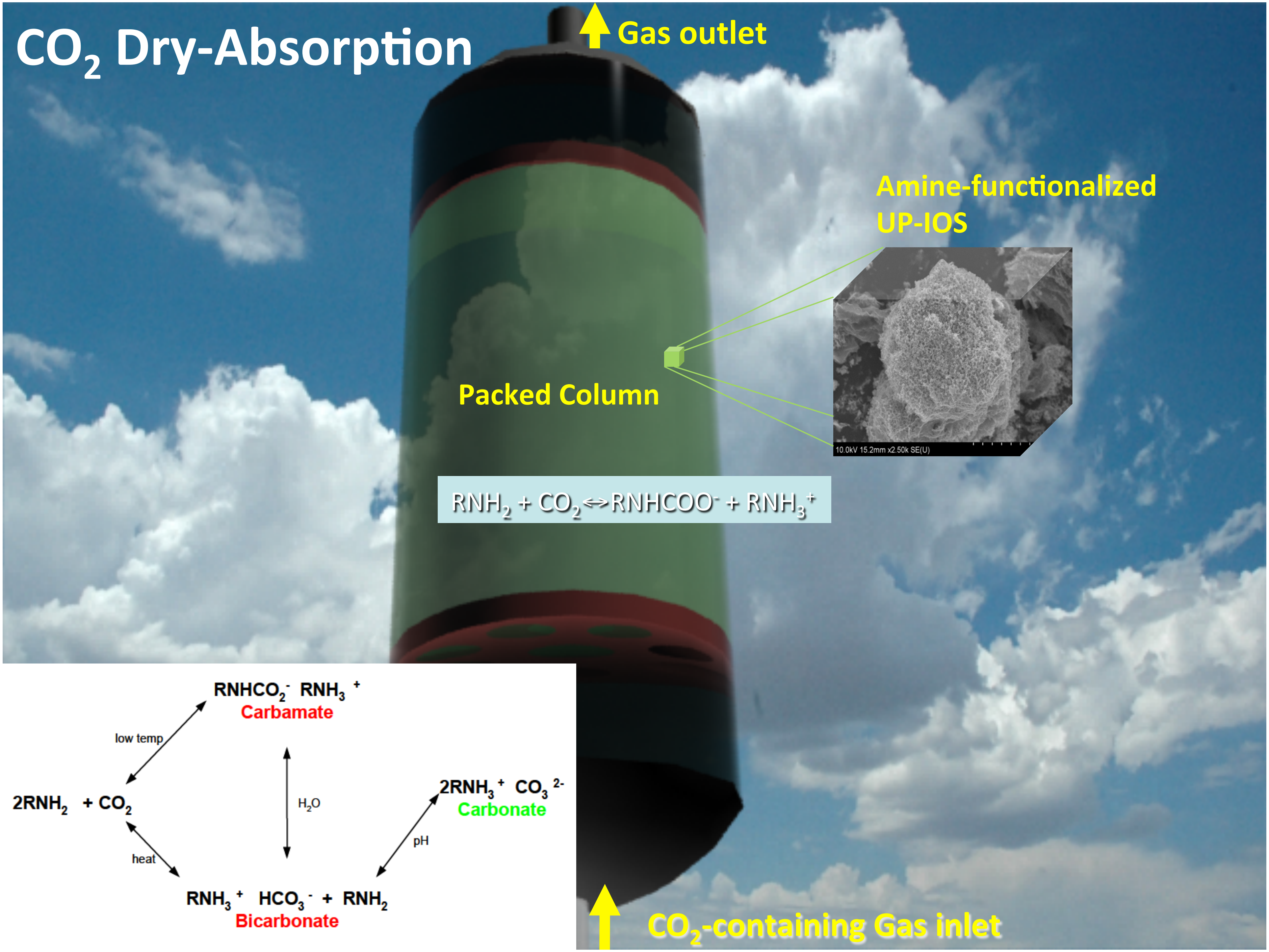
Bulk density: <0.05 g/cm^3
Specific area: ~ 600 m^2/g
Size: 50-500 μm

Packing material for absorption columns?

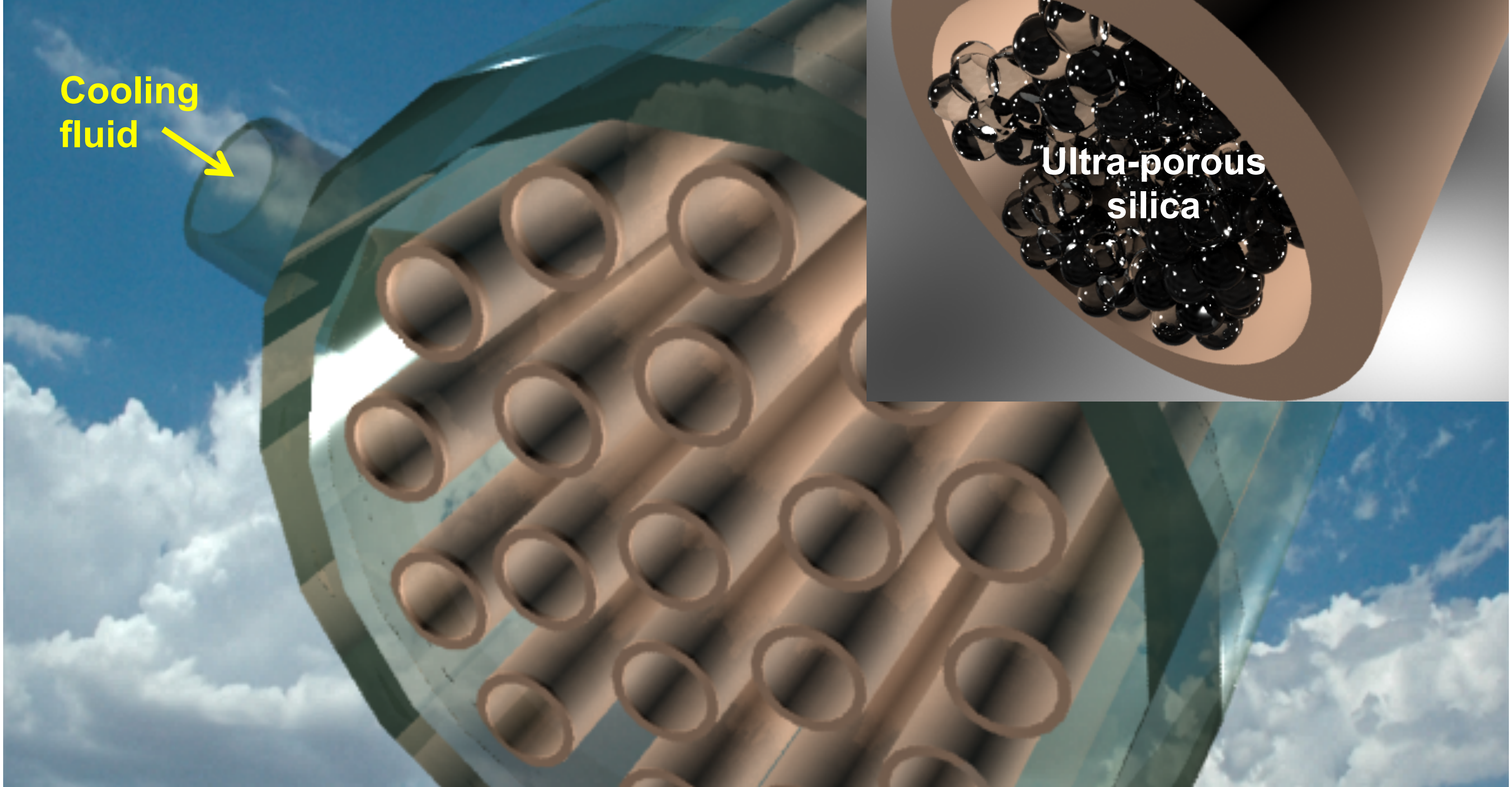
	Raschig rings	Intallox Sadlle	Pro-Pak	Silica Gel (Davisil® 643)	UP-IOS
Specific area (m^2/g)	7.4×10^{-4}	1.0×10^{-3}	3.3×10^{-3}	300	600

Sources: - Park et al. *Prepr. Pap.-Am. Chem. Soc. Div. Fuel Chem.* **2004**, 49 (1), 249.
- www.sigmaaldrich.com


CO_2 Dry-Absorption
Gas outlet
Amine-functionalized UP-IOS
10.0kV 15.2mm x2.50k SE(U)
Packed Column
$RNH_2 + CO_2 \leftrightarrow RNHCOO^- + RNH_3^+$
$RNHCO_2^-$ RNH_3^+
Carbamate
low temp
H_2O
$2RNH_2 + CO_2$
$2RNH_3^+$ CO_3^{2-}
Carbonate
pH
heat
RNH_3^+ HCO_3^- + RNH_2
Bicarbonate
CO_2-containing Gas inlet

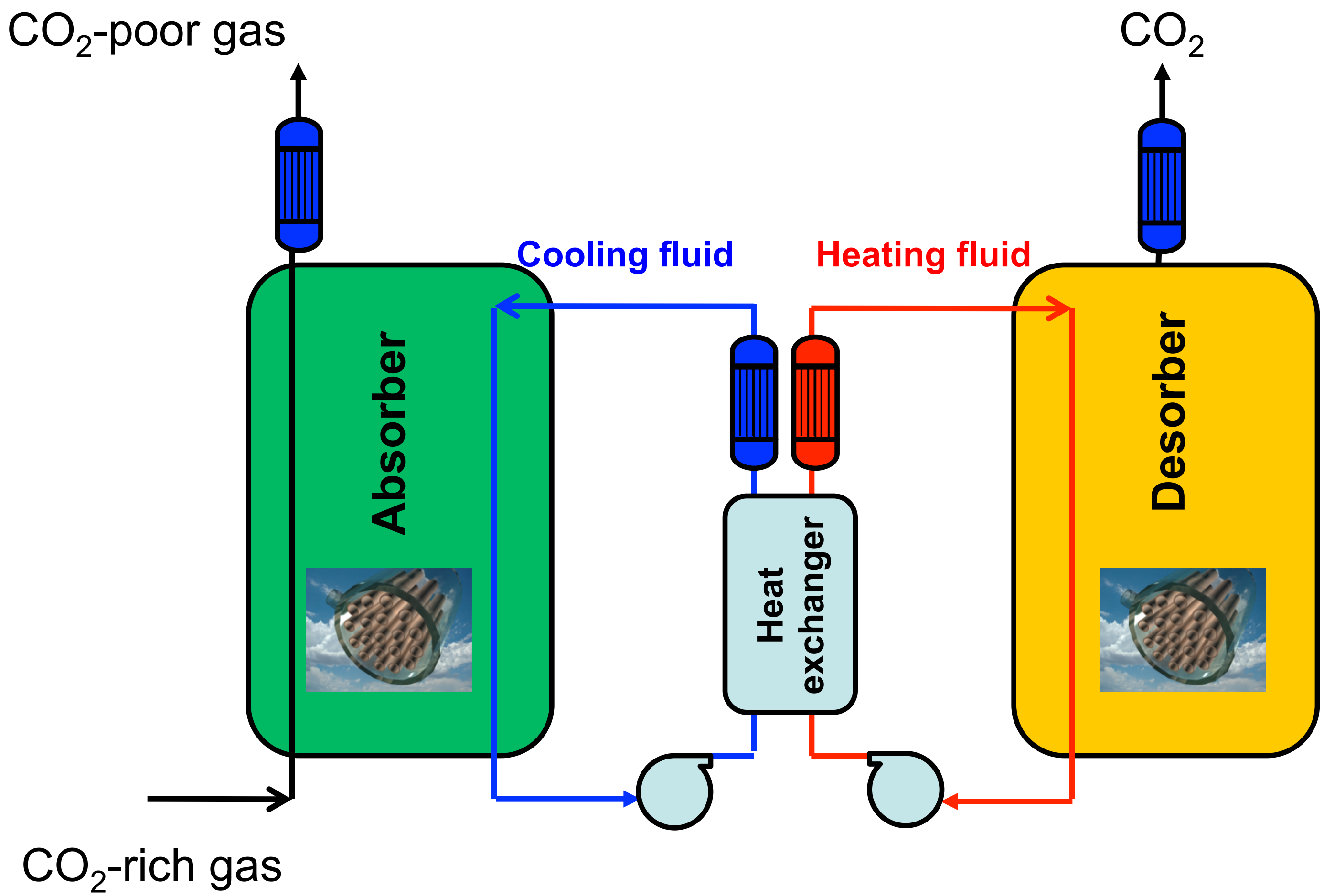
Micro-Absorbers



Absorption towers can be miniaturized using micro-tubes packed with ultra-porous inverse opal-like silica particles. Heat can be easily transferred to cooling fluid because of the huge transfer area.

Bundles of micro-absorbers can be used to prepare small, light disposable cartridges to be use in household or other small scale applications (sub-marines).

Absorption-Desorption Systems



Absorption-desorption systems can be inverted to regenerate the ultra-porous inverse-opal silica particles.

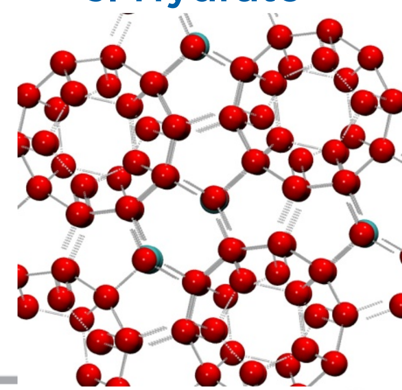
Sequestering CO_2 in the Seafloor

Multi-scale Modeling of CO_2 Hydrates (Jeff Klauda)

Scale	Sub-atomic	Molecular	Laboratory	Geological
Methods	Quantum Mechanics	Molecular Dynamics	Thermodynamic & Mass Transfer Modeling	Modeling with Field Data
Timescale	10^{-12} s	~10^{-5} s	Minutes to days	Years to Millennia

- Sub-atomic/Atomic-Level
  - Develop accurate guest-host potentials from high-level quantum mechanical methods[1]
  - Accurately describe CH_4/CO_2 adsorption in gas hydrate cavities
- Molecular-Level
  - Molecular dynamics simulations of CH_4/CO_2 hydrates
  - Compare crystal growth rates of these hydrates in equilibrium with water solution and gas (CH_4/CO_2) or liquid (CO_2)
  - Determine how pore structure and sediment type (clay/sand) influence crystal growth

sI Hydrate

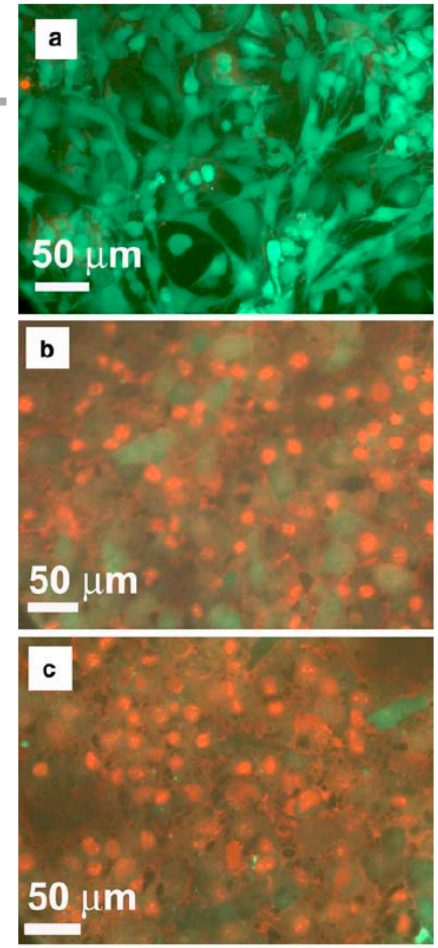


[1]Klauda and Sandler. *J. Phys. Chem. B*. 106: 5722 (2002).

Nanomaterials and Biological Barriers

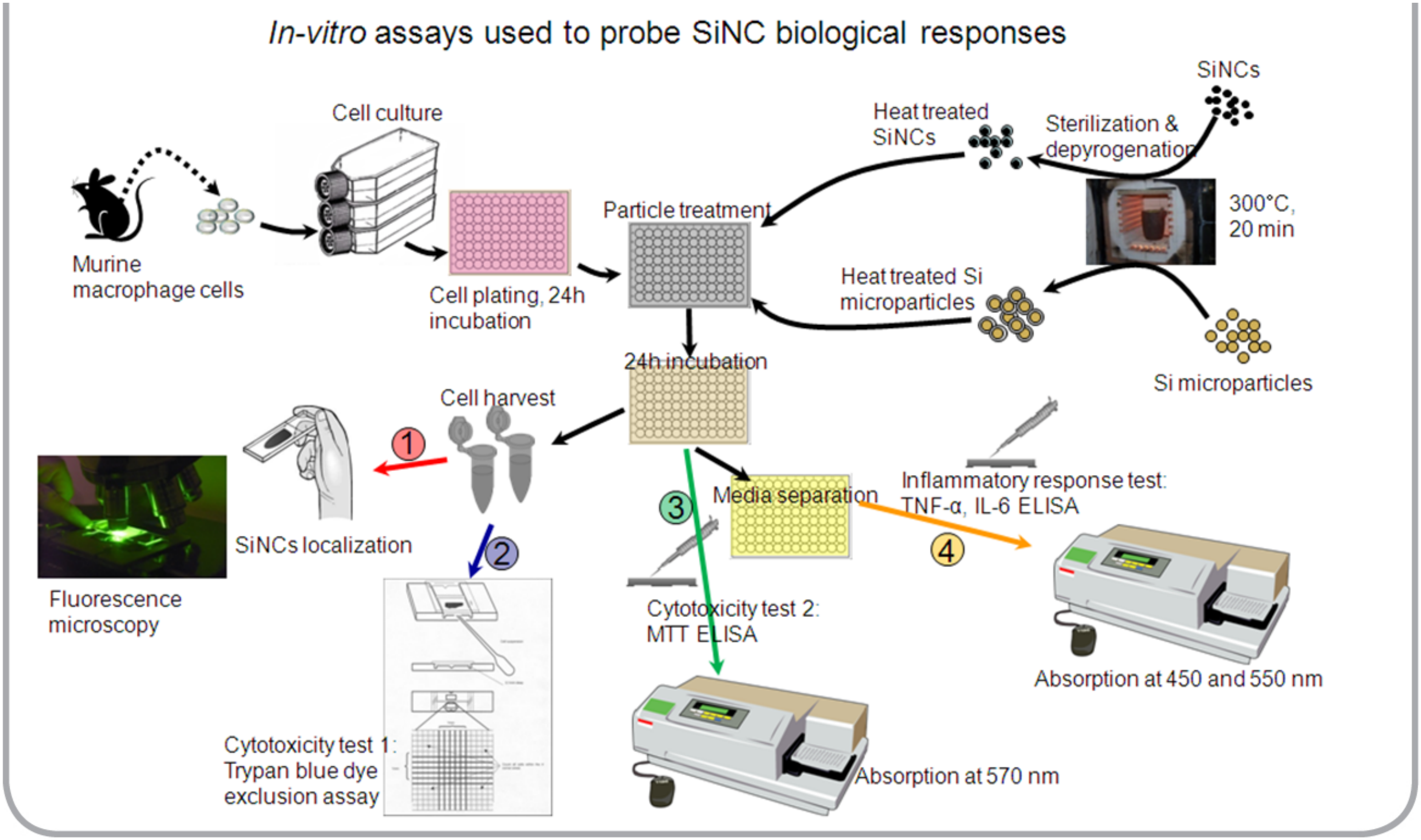
Srini Raghavan, ChBE
Nam Sun Wang, ChBE
Jeff Klauda, ChBE
Ganesh Sriram, ChBE
Sheryl Ehrman, ChBE
John Fisher, BIOE
Oded Rabin, MSE

Objectives:
(1) Systems level understanding of mechanisms of toxicity of nanomaterials
(2) Engineered materials for delivery of drugs, vaccines



Live/dead stain of chondrocytes cultured with a) silica NPs b) silica NPs + cisplatin and c) cisplatin Bhowmick et al., J Nanoparticle Research, in press, 2010

High throughput approach for rapid screening of toxicity, property/response relationships



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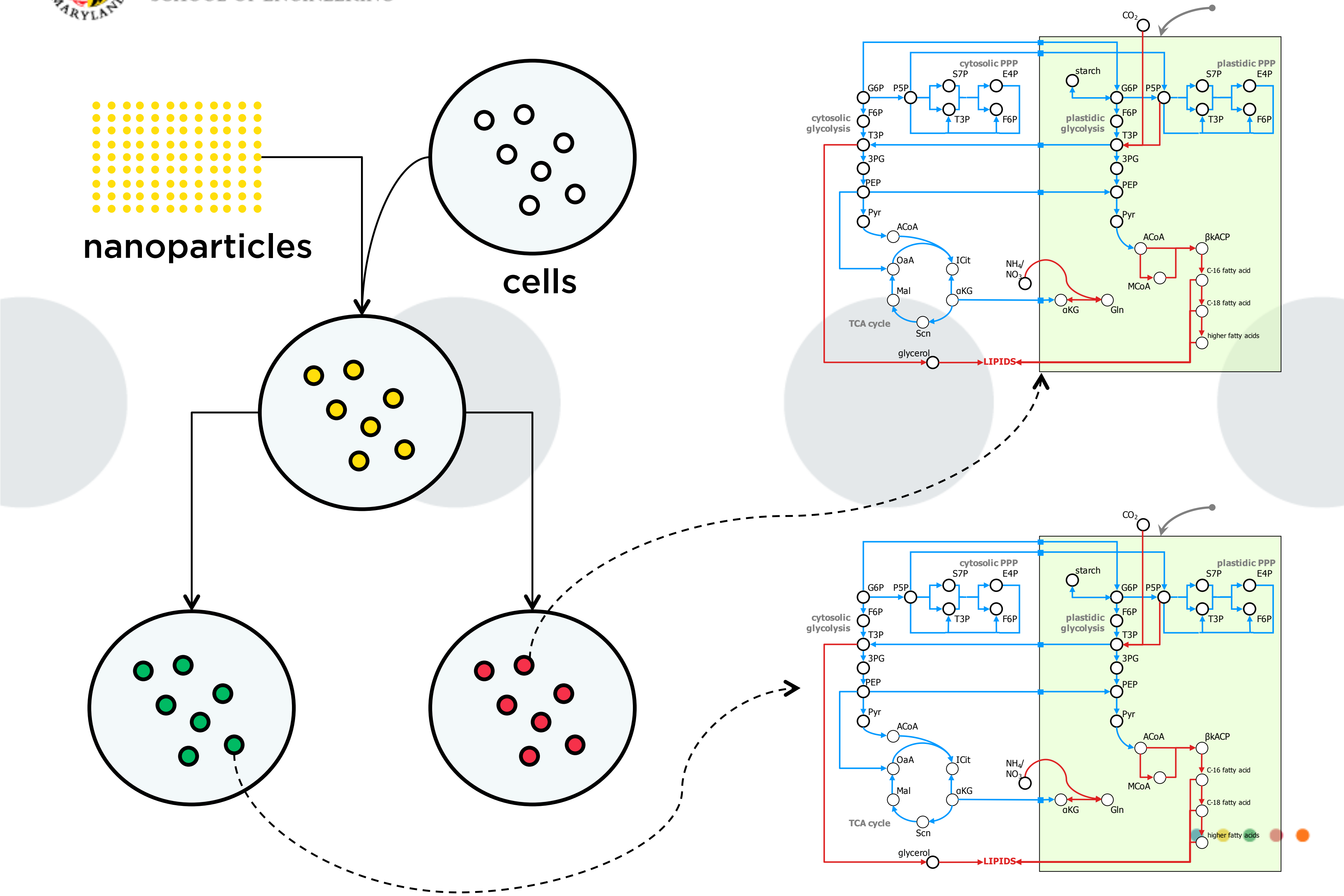
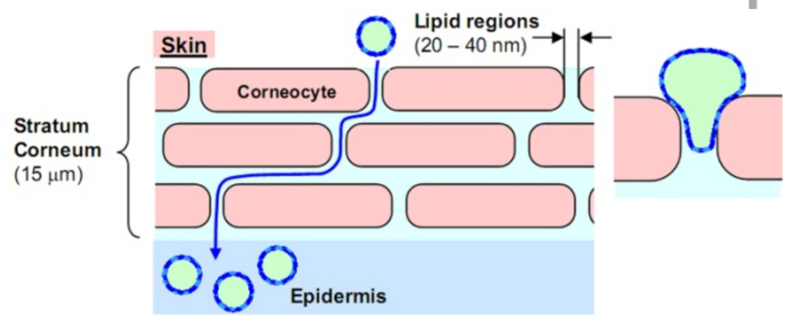
Systems bio approach:
Molecular understanding of toxicity mechanisms



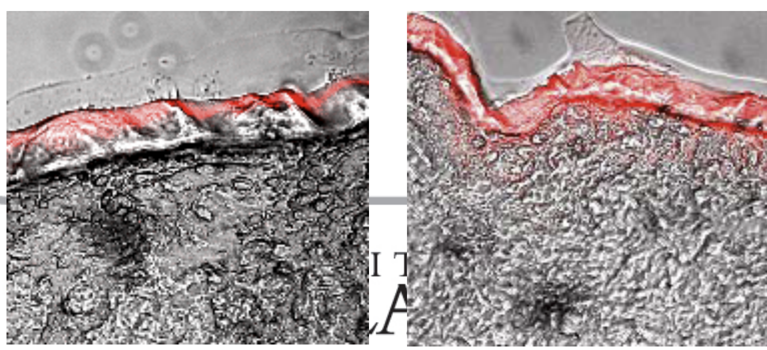
Delivery of Drugs, Vaccines, and Cosmetics by Liposomes

- **Skin Delivery**
  - Allows for delivery without ingestion or needles
  - Must cross the skin barrier to be delivered by the blood stream
  - Lipid/surfactant nanocontainers (liposomes) offer one route for skin delivery
  - These nanocontainers must first pass though the upper skin layer (stratum corneum)

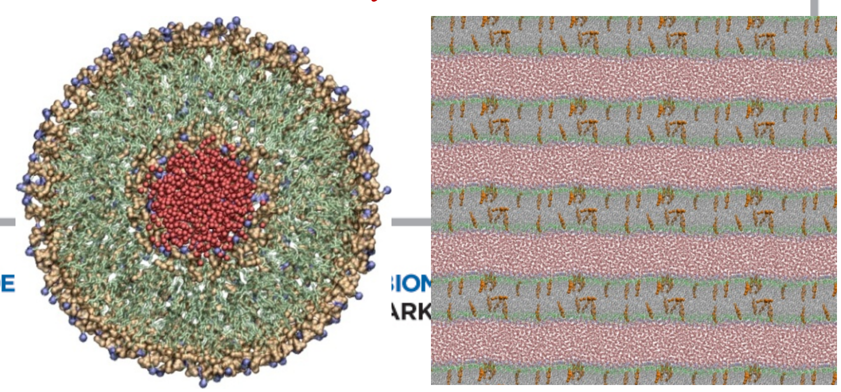


- **Traversing the Stratum Corneum**
  - Optimize liposome components to allow for penetration to the epidermis
  - Aim is to understand at a fundamental level how these liposomes move through the lipid pores of the stratum corneum

Fluorescently tagged Liposome Skin Transport
Dr. Srini Raghavan



Liposome and Skin Multilayer Molecular Simulations
Dr. Jeffery Klauda



Thanks!

For more information
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