Current Research Highlights
Biocatalysis and Biotechnology (BB)

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Department</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ping Wang*</td>
<td>BBE</td>
<td>Enzymology and biocatalysis, bioconversion and biosynthesis, biomaterials and functional coatings, bioelectrochemical processing, biosensors.</td>
</tr>
<tr>
<td>Mark Distefano</td>
<td>Chem</td>
<td>Organic and biochem., protein conjugates for therapeutic and biotechnology applications.</td>
</tr>
<tr>
<td>Mikael Elias</td>
<td>Biochem</td>
<td>Protein engineering and evolution, molecular modelling and recognition, bioremediation and quorum quenching strategies.</td>
</tr>
<tr>
<td>Wei-Shou Hu</td>
<td>CEMS</td>
<td>Systems biotechnology, biochemical engineering, cell culture bioprocessing, stem cell technology.</td>
</tr>
<tr>
<td>Romas Kazlauskas</td>
<td>Biochem</td>
<td>Biocatalytic synthesis of chemical intermediates and biofuels, enzyme modification for new reactions.</td>
</tr>
<tr>
<td>Lawrence Wackett</td>
<td>Biochem</td>
<td>Enzymes in biotechnology, immobilization technology, bioremediation, computer prediction tools for biocatalysis</td>
</tr>
<tr>
<td>Kechun Zhang</td>
<td>CEMS</td>
<td>Synthetic biology, metabolic engineering, protein engineering, biofuels, renewable chemicals.</td>
</tr>
</tbody>
</table>

*Program Leader (Email: ping@umn.edu; Phone: 612-624-4792)

Chemical and fuel bioprocessing; Biocatalyst engineering; Biotransformation and Bioremediation; Enzyme evolution; Bio-based polymers and biocoatings; Pathway engineering; Synthetic biology; Systems biotechnology; Cell culture bioprocessing
Enzymatic Protein Labeling

Mark Distefano is exploring how proteins accelerate chemical reactions and how proteins recognize other molecules with high specificity. This information is useful for drug design and biotechnology applications.

http://www.bti.umn.edu/faculty/biodistefano.html

Protein prenylation is a ubiquitous post-translational modification
Systems Design and Cell Engineering

Hu Lab

- Epigenomics
- Transcriptomics
- Proteomics
- Metabolomics
- Mathematical Modeling of Biological Reaction Network
- Parameter Estimation
- Simulation, Model Exploration
- Experimental Validation
- Model Prediction, Process Optimization

Genome engineering for biomanufacturing, genome technology for CHO cells

Biofilm and antibiotic resistance transmission, microbial invasion

E. faecalis

Chinese hamster

Stem cell engineering for hepatic applications, biomanufacturing, for cell therapy

Chinese hamster

iPSC
Protein Engineering

Ancestral catalyze new reactions

Reconstructed ancestral esterases and hydroxynitrile lyases are more promiscuous than modern enzymes

- engineers enzymes to be more stable, to have higher selectivity and even to catalyze new reactions.

http://www.umn.edu/~rjk
Nano Biocatalysis and Biomaterials

Conceiving and realizing nature-inspired multienzyme reaction pathways, Immobilized Biocatalysts, Bioproducts and Biopolymers, Bioenergy, Biosensors and Biomaterials.

http://www.bti.umn.edu/faculty/biowang.html
Bioproducts Innovations and Pathway Engineering

Our research program combines principles of chemistry, biology and engineering to achieve biosynthesis beyond nature.

http://www.cems.umn.edu/about/people/faculty.id21395.html
Biomedical and Pharmaceutical Materials (BPM)

Investigator | Department | Expertise
--- | --- | ---
Ron Siegel* | Phm\(^1\)/BME\(^2\) | hydrogels, drug delivery systems, microfabrication
Effi Kokkoli | CEMS\(^3\) | bioadhesion and drug targeting
Jayanth Panyam | Phm | multifunctional nanodelivery vehicles
Wei Shen | BME | bioactive materials
Calvin Sun | Phm | drug crystal and particle engineering
Raj Suryanarayanan | Phm | solid state properties of drugs, stability of drug/biomaterial formulations
Bob Tranquillo | BME/CEMS | fabrication and characterization of bioartificial cardiovascular replacement tissues
Chun Wang | BME | bio-molecular materials, polymer-based DNA and drug delivery, protein-based tissue scaffolds

*Program Leader (Email:siege017@umn.edu)

Affiliated Investigators: Chris Macosko,\(^3\) Marc Hillmyer,\(^4\) Theresa Reineke,\(^4\) Tom Hoye.\(^4\)

\(^1\)Pharmaceutics; \(^2\)Biomedical Engineering; \(^3\)Chemical Engineering and Materials Science, \(^4\)Chemistry

- Biomaterials for drug delivery, medical device coatings, and tissue engineering
- Drug/medical device combinations, characterization of drug/materials interactions
- Cell-based fabrication of bioartificial tissues
- Novel tissue mechanical testing and analysis methods
Inert Biodegradable Surfaces with “Artificial Mucus”

Efficient Release of Affinity-Captured Cells Using Coiled-Coil- Based Molecular Triggers

A label-free, affinity-based cell separation platform composed of a capture substrate and a cell-releasing molecular trigger. The capture substrate is functionalized with a capture antibody and a coiled-coil A. The cell-releasing molecular trigger B-PEG, a conjugate of coiled-coil B and polyethylene glycol, can drive efficient and gentle release of the captured cells. No excessive shear stress or enzymes are involved, and the released cells have neither external molecules attached nor endogenous cell-surface molecules cleaved, which might be critical for the viability, phenotype, and function of sensitive cells.

Wei Shen laboratory
Depending on the spacer used ssDNA-amphiphiles self-assemble into spherical micelles and bilayer nanotapes. The nanotapes progress from twisted nanotapes to helical nanotapes to nanotubes.

We can control the diameter and length of the ssDNA nanotubes, and we are exploring both ssDNA micelles and nanotubes for the targeted delivery of oligonucleotides.
Modulating Tabletability by Coating


Lab webpage: http://www.pharmacy.umn.edu/faculty/sun_changquancalvin/index.htm
<table>
<thead>
<tr>
<th>Investigator</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lorraine F. Francis*</td>
<td>Solidification, stress development, microstructure, printing</td>
</tr>
<tr>
<td>Satish Kumar*</td>
<td>Transport processes, interfacial phenomena, microfluidics</td>
</tr>
<tr>
<td>Marcio S. Carvalho**</td>
<td>Fluid mechanics, rheology, numerical methods</td>
</tr>
<tr>
<td>Alon V. McCormick</td>
<td>Curing, thermodynamics &amp; kinetics, NMR, stress development</td>
</tr>
<tr>
<td>C. Daniel Frisbie</td>
<td>Printing processes, printed electronics</td>
</tr>
<tr>
<td>Chris W. Macosko</td>
<td>Rheology, polymer processing</td>
</tr>
<tr>
<td>Xiang Cheng</td>
<td>Colloids, polymers, rheology, visualization</td>
</tr>
<tr>
<td>Michael Tsapatsis</td>
<td>Zeolite and particulate coatings, membranes, separations</td>
</tr>
<tr>
<td>Wieslaw Suszynski***</td>
<td>Coating process experiments, apparatus, flow visualization</td>
</tr>
</tbody>
</table>

*Program Co-Leaders

**Pontifica Universidade Catolica, Rio de Janeiro

***Research Engineer and Coating Process and Visualization Laboratory Manager
Coating of Rotating Discrete Objects with Complex Surface Geometry

**Challenge:** Non-uniform coating thickness due to surface curvature

**Model Problem**
Flow of a liquid film on *rotating cylinders*

- **Patterned Cylinders**
- **Slender Cylinders**
- **Increasing Film Thickness**
- **Increasing Rotation Rate**

- **Reverse Flows**
- **Film Rupture**
- **Liquid Shedding**

Smooth coatings will likely require simultaneous rotation and drying.

Weihua Li (Kumar)
Fabrication of an organic thin-film transistor (OTFT) by the SCALE process

Features of SCALE-processed OTFTs

- Charge carrier mobility: $0.8 \pm 0.4 \text{ cm}^2\text{V}^{-1}\text{s}^{-1}$
- On/off current ratio: $10^{5.3} \pm 0.3$
- Threshold voltage: $-0.3 \pm 0.0 \text{ V}$

A. Mahajan, W. J. Hyun (Frisbie, Francis)
Nanocrystal Coatings by Aerosol Jet Printing and Compaction

Objective

Develop continuous-amenable process for nanocrystal coatings

Results

Coating morphology depends on aerosol flow rate

Nanocrystal agglomerates form a continuous coating

Compaction increases density

Thermal annealing creates the desired microstructure

Bryce Williams (Francis, Aydil)

Williams et al. ACS Applied Materials & Interfaces 2015.
Goal: Study the effect of process conditions and die lip design on the trailing edge of patches coated with slot die.

Method: Solve the transient Navier-Stokes equations for free surface flows using the finite element method.

Main Result:

Minimized trailing edge on patches coated with slot coating process.


D. Maza (Carvalho)
Slot Coating of Particle Suspensions

Goal: Evaluate effect of particle concentration and size on process limits and particle distribution and orientation on the coated film.

Method: Solve the Navier-Stokes equations for free surface flows coupled with particle concentration and conformation transport equations using the finite element method.

Main Result:

Accurate prediction of process limits of particle suspension coating.

Effect of flow conditions on particle distribution and alignment on coated film.

Reboucas, Siqueira, Souza Mendes and Carvalho, JNNFM, sub., 2016

R. Reboucas and I. Siqueira (Carvalho)
Electronic Materials and Devices (EMD)

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Department</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steven Koester*</td>
<td>ECE (program leader)</td>
<td>Electronic devices, semiconductors</td>
</tr>
<tr>
<td>Chris Leighton</td>
<td>CEMS</td>
<td>Electronic/magnetic properties, film/layer growth</td>
</tr>
<tr>
<td>Paul Crowell</td>
<td>Physics</td>
<td>Magnetism, transport, ultra-fast spectroscopy</td>
</tr>
<tr>
<td>Steve Campbell</td>
<td>ECE</td>
<td>Thin-film photovoltaics, 2D materials</td>
</tr>
<tr>
<td>Bharat Jalan</td>
<td>CEMS</td>
<td>Complex oxides, molecular beam epitaxy</td>
</tr>
</tbody>
</table>

**Collaborators**

Andre Mkhoyan (CEMS), Dan Frisbie (CEMS), Xiaodong Xu (U. Washington), Ludwig Bartels (UCR), Chris Palmstrøm (UCSB), Chris Kim (ECE)

Synthesis, structural and chemical characterization of materials relevant for a wide range of electronic, optical and magnetic devices. Particular emphasis is placed on the understanding of the fundamentals of electronic structure and transport in electronic and magnetic materials, in addition to the materials science, physics and chemistry of the interfaces and nanostructures that play a vital role in device operation.
Understanding Electrolyte Gating to Understand Complex Oxides: $\text{La}_{0.5}\text{Sr}_{0.5}\text{CoO}_3-\delta$ (LSCO)

- Electrolytes can be used as unconventional gate dielectrics in transistors, generating unprecedented surface charge densities, and controlling electronic and magnetic properties. This has been studied here in LSCO.

- Temperature and gate bias windows for effective gating carefully established.
- Stark asymmetry in electrostatic vs. electrochemical gate response with bias polarity, with important implications for electrolyte gating of $n$-type vs. $p$-type oxides.
- Electrical control over transport, Curie temperature, etc., probed via anomalous Hall effect.

Heusler Alloy-Based Spintronic Devices

- Developing spintronic devices based on highly-polarized Heusler alloy ferromagnets integrated with semiconductors as well as high-Z metals (e.g. Pt):
  - Spin pumping devices
  - Microwave detection of spin accumulation
  - Spin injection from $\text{Co}_2\text{MnSi}$ and $\text{Co}_2\text{FeSi}$ into GaAs and detection at room temperature. Demonstration of spin pumping and large spin Hall magneto-resistance in heterostructures based on $\text{Co}_2\text{FeAl}/\text{Pt}$.
  - Heusler alloys have important applications in memory and logic applications as well as high-sensitivity magnetic sensors.

Novel Semiconductors

2D Materials

• Developed black phosphorus growth

S. A. Campbell, MRS, 2015.

• Developing growth system for transition metal dichalcogenides (TMDs):
  - Sulfides
  - Selenides
  - Heterojunctions

• Applications in flexible electronics and thin-film solar cells.

Photovoltaics

• Developed wide gap, low trap density CuInAlGaSe process

• Developed technique to control in-situ MoSe$_2$ orientation to prevent delamination

• Developed method for measuring interface trap density in materials with bulk traps

Campbell
SnS Nanosheets – Another “2D” Semiconductor?

- SnS is a 2D semiconductor with similar crystal structure to black phosphorus:

- Synthesized large (up to 10 µm wide and as thin as 3.5 nm) nanoplates. Raman / XRD consistent with orthorhombic SnS. → applications in optoelectronics and printed electronics.

research.cems.umn.edu/aydil
Graphene Coatings for Corrosion Protection

- Developed growth process for graphene directly on copper wires:
  - Used Tafel analysis to quantify corrosion rate in PBS electrolyte solution.
  - Demonstrated 10x reduction in corrosion rate compared to bare Cu.
  - Applications for medical electronics.

Q. Su and S. Koester, to be published.

Schematic diagram showing graphene-coated copper wire
## Flexible Electronics and Photovoltaics (FEP)

<table>
<thead>
<tr>
<th>Faculty Member</th>
<th>Department</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Russell J. Holmes</td>
<td>CEMS</td>
<td>Thin films, LEDs, solar cells</td>
</tr>
<tr>
<td>David Blank</td>
<td>CHEM</td>
<td>Ultrafast spectroscopy</td>
</tr>
<tr>
<td>Chris Douglas</td>
<td>CHEM</td>
<td>Molecular synthesis</td>
</tr>
<tr>
<td>C. Daniel Frisbie</td>
<td>CEMS</td>
<td>TFTs and printed electronics</td>
</tr>
<tr>
<td>P. Paul Ruden</td>
<td>ECE</td>
<td>Device modeling, transport theory</td>
</tr>
</tbody>
</table>

*Program Leader*

Interested in the design of materials, device architectures, and processes for the realization of flexible electronics and optoelectronics based on organic and hybrid organic-inorganic materials
Thermal gradient sublimation is used in industry to purify high value, small molecule organic semiconductors. Identified rate limited steps as transport down the tube to the deposition zone and a resistance to physical vapor deposition. Developed model has been used to optimize separation efficiency for multicomponent feeds and predict conditions for scale-up.

**Broad absorbing, cascade organic solar cells**

**PI: Holmes**

- SubPc and SubNc have complementary optical absorption
- Excitons are generated on both materials with transport occurring on SubNc – Energy cascade between SubPc and SubNc
- Diffusion on SubNc can be engineered via dilution

<table>
<thead>
<tr>
<th>Host</th>
<th>Acceptor</th>
<th>$\eta_P$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>$C_{60}$</td>
<td>2.0 ± 0.1</td>
</tr>
<tr>
<td>None</td>
<td>$C_{70}$</td>
<td>2.2 ± 0.1</td>
</tr>
<tr>
<td>UGH2 (Non-absorbing)</td>
<td>$C_{60}$</td>
<td>2.8 ± 0.1</td>
</tr>
<tr>
<td>SubPc</td>
<td>$C_{60}$</td>
<td>3.2 ± 0.1</td>
</tr>
<tr>
<td>SubPc</td>
<td>$C_{70}$</td>
<td>4.3 ± 0.2</td>
</tr>
</tbody>
</table>

Performance of host-guest cascade cell exceeds that of conventional devices that do not use a composite donor layer as well as those with a non-absorbing host.

New Approach for High-Resolution Printed Electronics

Inkjet-printed Ag ink is wicked into microimprinted channels on a plastic substrate, followed by a Cu electroless plating step. Ag metal inside the channel acts as a seed layer for selective deposition of Cu.

Major Process Attributes

- Line width and spacing down to 2 µm
- Conductivity 60% of bulk metal
- Additive
- Roll-to-roll compatible

R2R Nanoimprint at Minnesota

- Manufactured by Carpe Diem Technology
- Line Speed: 4-800 inches per minute
  - Web Width: 4-6 inches
Second R2R Line: Multimaterials, Slot, Gravure, Aerosol Jet

- Forward – reverse operation, multiple web paths
- Fully enclosed, HEPA filtered air
## Microstructured Polymers (MP)

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Department</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Frank S. Bates</td>
<td>CEMS</td>
<td>Thermodynamics, scattering, synthesis</td>
</tr>
<tr>
<td>Marc A. Hillmyer*</td>
<td>CHEM</td>
<td>Polymer synthesis and characterization (Director: Polymer Synthesis Facility)</td>
</tr>
<tr>
<td>Timothy P. Lodge</td>
<td>CHEM/CEMS</td>
<td>Polymer dynamics, solutions, scattering</td>
</tr>
<tr>
<td>Chris Macosko</td>
<td>CEMS</td>
<td>Rheology, processing</td>
</tr>
<tr>
<td>Mahesh Mahanthappa</td>
<td>CEMS</td>
<td>Synthesis, morphology, self-assembly</td>
</tr>
<tr>
<td>David C. Morse</td>
<td>CEMS</td>
<td>Theory and modeling</td>
</tr>
<tr>
<td>Theresa Reineke</td>
<td>CHEM</td>
<td>Biomedicine, Diagnostics, Targeted Delivery</td>
</tr>
</tbody>
</table>

**Collaborators include:**
Lorraine Francis (CEMS), Dan Frisbie (CEMS), Tom Hoye (CHEM), Chris Leighton (CEMS), Ron Siegel (PHRM), Bill Tolman (CHEM)

*Program Leader*

**Synthesis, characterization, dynamics, processing, properties, and theory**
Toughening Poly(lactide) with Block Copolymer Micelles

- Low molecular weight poly(ethylene oxide)-b-poly(butylene oxide) (EB) diblock copolymer forms micelles in poly(L-lactide) (PLLA).
- Dispersion of micelles in PLLA is due to a negative $\chi$ parameter between poly(ethylene oxide) and PLLA.
- Micelles impart outstanding impact and tensile toughness at relatively low loadings without compromising modulus, $T_g$ or optical clarity.

Tuoqi Li, Jiuyang Zhang, Deborah K. Schneiderman, Lorraine Francis and Frank S. Bates (ACS Macro Letters 2016)
Catalyst Localized at Interface in Polymer Blends

90 / 10 HDPE / PLA

$\text{d} = 0.77 \pm 0.20 \ \mu\text{m}$

60 / 30 / 10 / 0.4 HDPE / HO-PE-OH / PLA / SnOct$_2$

$\text{d} = 0.26 \pm 0.04 \ \mu\text{m}$

TEM + EDS

Sn Sn L$\alpha$, L$\beta$

Counts

Energy (eV)

2000 3000 4000 5000

Thurber Lodge, Macosko, *ACS Macro Letters*, 2015, 1, 30-33
Versatile ion gels for plastic electronics

ABA triblock copolymers swollen with ionic liquids are excellent candidates for organic transistor gate dielectrics, polymer gel electrolytes, and luminescent devices, among others. This versatility stems from a combination of attributes, including tunable mechanical strength, high throughput printability, high ionic conductivity, high capacitance, and thermal stability.

Electrochromic ion gel operating at only 1 V. Methyl viologen is the chromophore, in an ion gel containing PS-PMMA-PS and [EMI][TFSI]
(H. C. Moon)

Photoreversible ion gel consisting of P(NIPAm-ran-AzoMA)-PMMA-P(NIPAm-ran-AzoMA) in [EMI][PF₆], operating under alternating UV and visible irradiation (T. Ueki)

PCHE–PEO Block Polymer for Metal Oxide Templating

Approach

• Anionic polymerization and hydrogenation for the synthesis of new block polymer PCHE–PEO
• PEO selectively imbibes sol-gel reactants/metal ions

Outcome

• Large $\chi$ enabled self-assembly at low $N$
• Formation of ultra-small particles (6 ± 1 nm)
• Versatile templating of silica, iron oxide, titania

1. Solvent anneal PCHE–PEO Film
2. Selectively Deposit Inorganic Precursors within PEO domain
3. Oxidize Inorganic and Remove BP Template

Schulze, Sinturel, & Hillmyer
ACS Macro Lett., 4, 1027, 2015

Elastomers and PSAs from Isosorbide-Based Block Polymers


University of Minnesota, Department of Chemistry

BTCBA, AIBN
70 °C, 2 h

AAI, AIBN
DMF, 70 °C, 2h

<table>
<thead>
<tr>
<th>Polymer</th>
<th>$M_n$, th. (kg/mol)</th>
<th>$M_n$, SEC (kg/mol)</th>
<th>$M_n$, NMR (kg/mol)</th>
<th>$D$</th>
<th>wt% PAAI (NMR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAAI-PnBA-PAAI (53k, 12%)</td>
<td>51.7</td>
<td>53.3</td>
<td>49.8</td>
<td>1.09</td>
<td>12</td>
</tr>
<tr>
<td>PAAI-PnBA-PAAI (60k, 17%)</td>
<td>56.1</td>
<td>60.2</td>
<td>65.6</td>
<td>1.12</td>
<td>17</td>
</tr>
<tr>
<td>PAAI-PnBA-PAAI (70k, 21%)</td>
<td>59.5</td>
<td>69.2</td>
<td>67.5</td>
<td>1.15</td>
<td>21</td>
</tr>
</tbody>
</table>
# Nanostructural Materials and Processes (NMP)

<table>
<thead>
<tr>
<th>Investigator</th>
<th>Department</th>
<th>Expertise</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alon McCormick</td>
<td>CEMS</td>
<td>Materials and Emulsions Synthesis; Spectroscopy and CryoMicroscopy</td>
</tr>
<tr>
<td>C. Daniel Frisbie</td>
<td>CEMS</td>
<td>Molecular Materials and Interfaces; Molecular Electronics</td>
</tr>
<tr>
<td>Wayne Gladfelter</td>
<td>CHEM</td>
<td>Materials Chemistry; Inorganic Chemistry; Scanning Probe Microscopy</td>
</tr>
<tr>
<td>Christy Haynes</td>
<td>CHEM</td>
<td>Porous and plasmonic nanomaterials, nanoparticle toxicity</td>
</tr>
<tr>
<td>Greg Haugstad</td>
<td>CHARFAC</td>
<td>AFM Scanning Probe Microscopy</td>
</tr>
<tr>
<td>R. Lee Penn</td>
<td>CHEM</td>
<td>Environmental Solid State Chemistry</td>
</tr>
<tr>
<td>Ilja Siepmann</td>
<td>CHEM</td>
<td>Predictive Modeling of Phase and Sorption Equilibria</td>
</tr>
<tr>
<td>Andreas Stein</td>
<td>CHEM</td>
<td>Solid State Chemistry of Porous Materials</td>
</tr>
<tr>
<td>Michael Tsapatsis</td>
<td>CEMS</td>
<td>Materials Synthesis, Structure Elucidation</td>
</tr>
<tr>
<td>Joe Zasadzinski</td>
<td>CEMS</td>
<td>Microscopy of Complex Fluids</td>
</tr>
</tbody>
</table>

**Associated Investigators:**
Frank Bates, Lorraine Francis, Eric Kaler, Chris Macosko, Wei Zhang

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*synthesis, phase behavior, structure, and performance of surfactants and self-assembled molecular and colloid systems*
In situ colloid probe AFM: “Hyperspectral” force mapping methods (here on crosslinked, oriented fibrin gel) Haugstad (Anne Ellis, Bob Tranquillo)

Contact-mode height image... *interlaced* with force spectroscopy (steric, “frictionless” contact)

Elasticity histogram

Hertzian model
$R = 3.3 \text{ um probe}$
$k = 0.08 \text{ N/m cantilever}$

Elasticity histogram

Goal: Quantify mechanical anisotropy

Need: hyperspectral dataset analysis (large)

Guido and Tranquillo, “A methodology for the systematic and quantitative study of cell contact guidance in oriented collagen gels...”, *J Cell Sci*, 1993
Morin and Tranquillo, “Guided sprouting from endothelial spheroids in fibrin gels aligned by magnetic fields and cell-induced gel compaction”, *Biomaterials*, 2011
Dispersion processes (McCormick group with *collaborators*)

1. Cryo-EM Monitoring

Example of nanoemulsion with non-ionic surfactant

![Image of nanoemulsion with non-ionic surfactant](image1.png)


Sphere (ellipsoids) to cylinder transition

![Image of sphere to cylinder transition](image2.png)


2. Surfactant mixtures for dispersion

Example: Span 80 effect on crude oil dispersion

![Image of surfactant mixture effect on crude oil dispersion](image3.png)

Characterizing the dynamics of aggregation in reactive systems (PENN)

$U_{60}$ clusters in water
*Soltis et al., JACS, 2016*

WATER: after aging.
*Yuwono, Burrows, Soltis, Penn (JACS, 2010)*

pH 3.5

Yuwono, Burrows, Soltis, *Penn* (*Faraday Trans 2012*)

WATER

pH 5.5

CRYO-TEM images of nanoparticles in liquid media.

Isopropanol
*Burrows, Talmon, Penn; 2013*

Tetrahydrofuran
Discovery of Zeolites for Sweetening of Sour Natural Gas

- Hierarchical screening of all known zeolites for binary H₂S/CH₄ and H₂S/C₂H₆ mixtures and of 16 top-performing zeolites for four- and five-component mixtures
- Simulations yield direct information on selectivity, capacity & number of adsorption stages


Understanding Transport in Hierarchical Zeolites

- MD elucidate the complex diffusion of sorbates in house-of-cards nanosheets where the large free energy penalty for transfer from micropores to mesopores leads to a tortuous diffusion pathway

Bai, ..., Tsapatsis & Siepmann, ACS Nano, submitted

Sensitivity of Nucleation Free Energies to Force Fields

- This work demonstrates that the sensitivity of predicted nucleation rates to details of the molecular models can be dramatically reduced by comparing nucleation at the same relative state point

Stein Group: Nanostructured & Nanoporous Materials

Stabilizing metal-organic frameworks for high temperature catalysis


All-solid-state potentiometric ion-sensing platform


Novel high capacity Li-ion battery cathode materials


Modified GO materials for improving fracture toughness at very low loadings