<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
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**

- **Enterococcus faecalis**

- **Chinese hamster iPSC**

- **Stem cell engineering for hepatic applications, biomanufacturing, for cell therapy**
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
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)

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

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

Affiliated Investigators:  
- Chris Macosko\(^3\), Marc Hillmyer\(^4\), Theresa Reineke\(^4\), Tom Hoye\(^4\)
- Pharmaceutics;  
- Biomedical Engineering;  
- Chemical Engineering and Materials Science;  
- 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

1. Addition of a cell mixture on the capture substrate.
2. Capture of target cells.
3. Washing of non-target cells.
4. Release of captured cells using the molecular trigger B-PEG.

Selective capture of endothelial cells
Efficient release of the captured endothelial cells by B-PEG

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
Spacer between single stranded DNA (ssDNA) and hydrophobic tail affects self-assembly, secondary structure and binding.

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

PL: Changquan Calvin Sun
sunx0053@umn.edu


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

**Pontifical 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

Imposed Surface Topography & Complex Cross-section Shape

Reverse Flows
Increasing Film Thickness
Trapping of liquid may be detrimental to coating quality

Patterned Cylinders

Increasing Rotation Rate

Slender Cylinders
Film Rupture
Liquid Shedding

Smooth coatings will likely require simultaneous rotation and drying

Weihua Li (Kumar)
**Self-Aligned Capillarity-Assisted Lithography for Electronics (SCALE)**

- **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)**
**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.
Coating Patches: Analysis of Shutdown Process

**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.

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
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>
<tr>
<td>Renata Wentzcovitch</td>
<td>CEMS</td>
<td>Electronic structure theory</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.
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 injection from Co$_2$MnSi and Co$_2$FeSi into GaAs and detection at room temperature. Demonstration of spin pumping and large spin Hall magneto-resistance in heterostructures based on Co$_2$FeAl/Pt.

- Heusler alloys have important applications in memory and logic applications as well as high-sensitivity magnetic sensors.


Microwave detection of spin accumulation

Spin pumping devices
Novel Semiconductors

2D Materials

- Developed black phosphorus growth
- Developing growth system for transition metal dichalcogenides (TMDs):
  - Sulfides
  - Selenides
  - Heterojunctions

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

- Applications in flexible electronics and thin-film solar cells.
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.
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.
**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
Purification of specialty electronic materials

PI: Cussler, Holmes and Dow Chemical Co.

• 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

Performance at an intensity of 100 mW/cm² under AM 1.5G solar simulated illumination

<table>
<thead>
<tr>
<th>Host</th>
<th>Acceptor</th>
<th>$\eta_p$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>None</td>
<td>C₆₀</td>
<td>2.0 ± 0.1</td>
</tr>
<tr>
<td>None</td>
<td>C₇₀</td>
<td>2.2 ± 0.1</td>
</tr>
<tr>
<td>UGH₂</td>
<td>C₆₀</td>
<td>2.8 ± 0.1</td>
</tr>
<tr>
<td>SubPc</td>
<td>C₆₀</td>
<td>3.2 ± 0.1</td>
</tr>
<tr>
<td>SubPc</td>
<td>C₇₀</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

**PI: Frisbie and Francis (CPF)**

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
<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</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(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

![5 wt% EB-1](image)

**Izod impact strength**

![Tensile strength](image)

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

\[ d = 0.77 \pm 0.20 \, \mu m \]

90 / 10 HDPE / PLA

\[ d = 0.26 \pm 0.04 \, \mu m \]

60 / 30 / 10 / 0.4 HDPE / HO-PE-OH / PLA / SnOct_2

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 ($6 \pm 1$ 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

\[
\begin{align*}
\text{BTCBA, AIBN} & \quad 70 \degree C, 2 \text{ h} \\
\text{AAI, AIBN} & \quad \text{DMF, } 70 \degree C, 2 \text{ h}
\end{align*}
\]

<table>
<thead>
<tr>
<th>Polymer</th>
<th>(M_n, \text{th.} ) (kg/mol)</th>
<th>(M_n, \text{SEC} ) (kg/mol)</th>
<th>(M_n, \text{NMR} ) (kg/mol)</th>
<th>(\hat{D} )</th>
<th>wt% PAAI (NMR)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PAAI-PnBA-PAAI</td>
<td>51.7</td>
<td>53.3</td>
<td>49.8</td>
<td>1.09</td>
<td>12</td>
</tr>
<tr>
<td>(53k, 12%)</td>
<td></td>
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<tr>
<td>PAAI-PnBA-PAAI</td>
<td>56.1</td>
<td>60.2</td>
<td>65.6</td>
<td>1.12</td>
<td>17</td>
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<tr>
<td>(60k, 17%)</td>
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<tr>
<td>PAAI-PnBA-PAAI</td>
<td>59.5</td>
<td>69.2</td>
<td>67.5</td>
<td>1.15</td>
<td>21</td>
</tr>
<tr>
<td>(70k, 21%)</td>
<td></td>
<td></td>
<td></td>
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</tbody>
</table>

PSA Peel Test

![PSA Peel Test Graph](image)
## Nanostructural Materials and Processes (NMP)

<table>
<thead>
<tr>
<th>Investigator</th>
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</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>Greg Haugstad</td>
<td>CHARFAC</td>
<td>AFM Scanning Probe Microscopy</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(Director, Characterization Facility)</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, Christy Haynes, Eric Kaler, Chris Macosko, Wei Zhang

*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)
- Hysteresis: modulus correlation
- 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


Sphere (ellipsoids) to cylinder transition


2. Surfactant mixtures for dispersion

Example: Span 80 effect on crude oil dispersion

![Graph showing interfacial tension and effectiveness of Span 80](image)

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)

pH 5.5

CRYO-TEM images of nanoparticles in liquid media.

Isopropanol
Burrows, Talmon, Penn; 2013

Tetrahydrofuran
Predictive Modeling of Separation Processes and Nanostructured Materials– Siepmann

**Funding from NSF (CBET, CHE, SI2), DOE (MGI, SciDAC, EFRC, EERE), Industry & IPRIME**

**Discovery of Zeolites for Sweetening of Sour Natural Gas**
- Hierarchical screening of all known zeolites for binary \(\text{H}_2\text{S}/\text{CH}_4\) and \(\text{H}_2\text{S}/\text{C}_2\text{H}_6\) 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**

www.chem.umn.edu/groups/stein  
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(612) 624-1802

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**Stabilizing metal-organic frameworks for high temperature catalysis**


**All-solid-state potentiometric ion-sensing platform**


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**Novel high capacity Li-ion battery cathode materials**


**Modified GO materials for improving fracture toughness at very low loadings**

Qian et al., PCT Int. Appl. 2015, WO 2015184223 A1  
20151203. PCT Int. Appl. 2014, WO 2014143758 A2 20140918
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Ryo Katayama
Asahi Kasei

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Effect of drying conditions on particle distribution

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**Research Project**  
**Film formation and stress development**