Research Highlights
Nanostructural Materials and Processes
NMP
## Nanostructural Materials and Processes (NMP)

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<tr>
<th>Investigator</th>
<th>Department</th>
<th>Expertise</th>
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<tr>
<td>Alon McCormick</td>
<td>CEMS</td>
<td>Materials and Emulsions Nanostructure, CryoMicroscopy</td>
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<td>C. Daniel Frisbie</td>
<td>CEMS</td>
<td>Molecular Materials and Interfaces; Molecular Electronics</td>
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<tr>
<td>Wayne Gladfelter</td>
<td>CHEM</td>
<td>Materials Chemistry; Inorganic Chemistry; Scanning Probe Microscopy</td>
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<tr>
<td>Greg Haugstad</td>
<td>CHARFAC</td>
<td>AFM Scanning Probe Microscopy (Director, Characterization Facility)</td>
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<td>Christy Haynes</td>
<td>CHEM</td>
<td>Interface of Bioanalytical and Biomaterials Chemistry</td>
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<td>R. Lee Penn</td>
<td>CHEM</td>
<td>Environmental Solid State Chemistry</td>
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<td>Ilja Siepmann</td>
<td>CHEM</td>
<td>Predictive Modeling of Phase and Sorption Equilibria</td>
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<td>Andreas Stein</td>
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<td>Solid State Chemistry of Porous Materials</td>
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<td>Michael Tsapatsis</td>
<td>CEMS</td>
<td>Materials Synthesis, Structure Elucidation</td>
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<td>Joe Zasadzinski</td>
<td>CEMS</td>
<td>Microscopy of Complex Fluids</td>
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**synthesis, phase behavior, structure, and performance of surfactants and self-assembled molecular and colloid systems**
Unravelling Tin Precursor Deposition Chemistry Using Computational Methods

Wayne L. Gladfelter, Chemistry, Bharat Jalan, CEMS, Christopher Cramer, Chemistry

Tin oxide films by CVD
Low emissivity windows
Transparent conducting oxides
Sensors of combustible gases and CO

Tin-containing perovskites (e.g. BaSnO₃)
High temperature power devices
All perovskite, transparent electronics
High mobility 2-D electron gas films

Graph showing mole fraction vs temperature with various SnMe₄ isomers and SnMe₃ isomers.
Analytical & Biomedical Applications of Nanomaterials
Based on Silica Platform - Haynes Group

Improved Tissue Cryopreservation using Nanowarming: Inductive Heating of Magnetic Nanoparticles

Perfluorocarbon-Loaded Mesoporous Silica Nanoparticles as NMR Sensors of Abiotic Factors

Silica-coated, pH-sensitive Swelling Polymer for Drug Delivery Applications

The Effect of Surface Charge Density of Silica Nanoparticles on the Interaction with Bacteria

Shewanella oneidensis
Dispersion and nanostructural mechanisms (McCormick & collaborators)
research.cems.umn.edu/mccormick

Making vesicles, liposomes, etc.

Surfactant blends for rapid dispersion
DOSS/Tween89/Span80 and Lecithin/Tween80
Crude oil in Sea water

Riehm
Rokke Paul Vizanko
Lee


Currently also
Raghavan (Maryland),
John (Tulane), Bothun
(U Rhode I),
Corcoran
Penn

Wear of nanostructured coatings
Hubig (Ecolab) Riehm Lee Haugstad Suszynski Luo

Hydration & wear of hydrogel coatings
Colling
Zeng
(Boston Scientific)
Wormuth
Haugstad

Simulating micelle dynamics
Mysona Morse
APS March Meeting 2017
Simulation of Dynamical Processes in Block Copolymer Micelles
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

Thermodynamics of Olefin Oligomer Blends
Extrapolation of data from simulations of oligomers allows to predict properties of polymers
Chen, ..., Lodge & Siepmann, Macromolecules 49, 3975 (2016)

Accelerated Computational Analysis of Metal–Organic Frameworks for Oxidation Catalysis
Hierarchical screening of CoRE (computation-ready experimental) MOF database to find frameworks with accessible high-spin iron(IV)-oxo nodes with potential for selective catalysis of ethane to ethanol
Vogiatzis, ..., Siepmann & Gagliardi, J. Phys. Chem. C 120, 18707 (2016)

Structure and Phase Behavior of Mixed Self-Assembled Alkanethiolate Monolayers on Gold Nanoparticles
Simulations demonstrate that alkanethiolates of different lengths tend to segregate into domains (Janus particles) on the same nanoparticle
Nanostructured & Nanoporous Materials - Stein group

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Solid Adsorbents for Removal of Dilute H₂S from Claus Tail Gas
(With M. Tsapatsis)

Renewable Electricity by High Energy Advanced Thermal Storage
(with J. Davidson, I. Siepmann)

Stabilizing metal-organic frameworks for high temperature catalysis
(with R.L. Penn, C. Lu and many ICDC collaborators)

All-solid-state potentiometric ion-sensing platform
(with P. Buhlmann)

Modified GO materials for improving fracture toughness at very low loadings
(with C. Maccosko, E. Tadmor)

Novel high capacity Li-ion battery cathode materials
(with D. Truhlar)
Interfacial Dilatational Viscosity

A. Sachan, S. Patton, C. Valtierrez-Gaytan, B. Stottrup, and J. Zasadzinski

https://sites.google.com/a/umn.edu/zasadzinski/

Interfacial Dilatational Rheometer

Laplace equation
\[ g = \frac{(P_{in} - P_{out})R}{2} \]

Phase separation, phase continuity and bubble curvature all play roles in dilatational modulus