

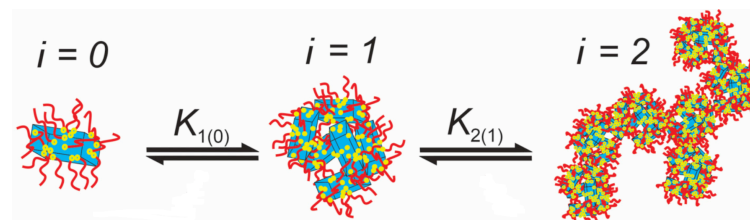
The Center for Hierarchical Emergent Materials (CHEM)



CHEM seeks to understand, control and predict the assembly of multi-hierarchical materials of industrial relevance. Reinforced elastomers, paints, inks, biomaterials, surfactants, detergents and coacervates, semi-crystalline polymers, block copolymers, catalysts, filters, membranes, skin. Time dependence in processing/application, 4D.

Synergy: Dynamic and static properties understood for one field of application could be adapted to another field. Rheology simulation methods from polymers to detergents to paints.

Parallelism and Convergence: Similar solutions for different applications. Aggregate pigments and aggregate reinforcing fillers both rely on micron-scale networks in application.



Center Proposition

- We understand chemistry/molecular scale
- We understand processing and the macroscopic
- How do materials self-assemble from the chemistry and nano-level to the macroscopic in processed industrial materials?*



Paint is composed of a dispersion of nanoparticles that self assemble during processing, application and during drying to present the final color, translucency, brilliance. The process is complex. The issues involved are multiscale and hierarchical involving rheology, morphology, chemistry, kinetics. There are many parallel industrial problems involving hierarchical emergence for inks, reinforced elastomers, printed electronics, detergents, coacervates, biomimetic and biological systems.



The Center for Hierarchical Emergent Materials (CHEM)



Greg Beaucage, Scattering,
Nanocomposites,
Pigments

Yoonjee Park, Skin/Surfactants,
Biomed delivery

Jon Nickels, Scattering,
Aqueous Systems

Neil Ayers, Synthesis,
Polymers,
Surfactants,
Surfaces



Dave Martin, Microscopy,
Conjugated
Polymers,
Crystalline
Structure

Arthi Jayaraman, Simulation,
Polymer Grafted
Nanoparticles

Darrin Pochan, Surfactants,
Polymers,
Microscopy

Norm Wagner, Rheology,
Scattering

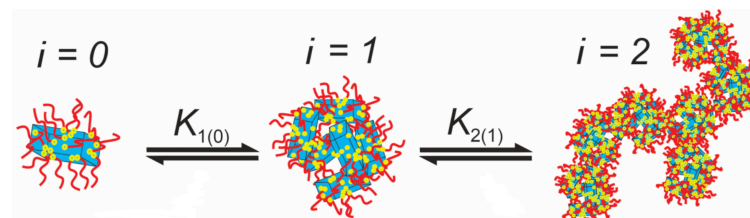


Anish Tuteja, Surfaces,
Dispersion

Nick Kotov, Complex
Hierarchies

Ron Larson, Rheology,
Simulation

Jinsang Kim, Synthesis,
Polymers,
Biomedical,
Sensors



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Thrust I. Emergent Particulate Hierarchies



Materials such as paints, inks, filled polymers, and reinforced elastomers involve immiscible, generally aggregated, polydisperse particles which are often on the nanoscale which assemble through processing, application, and time into useful structures often reflecting a network such as a filler network or pigment network on the micron to macro-scale.

This thrust also involves engineered and controlled nanostructural particulates targeting specific design targets such as the work of Nick Kotov.

Thrust III. Surface Engineering, Coatings, and Adhesives



This thrust focuses on the manipulation of surfaces in terms of interaction with the environment such as hydrophilicity, oleophilicity, biocompatibility. Coatings and adhesives are topics of interest.

Thrust V. Surfactants and Coacervates



Emergent hierarchical structures in surfactant systems.

Thrust II. Materials Data Science



This thrust involves development of tools to utilize large data sets towards targeted goals involving formulation chemistry targeting hierarchical emergence. This Thrust will be in collaboration with the University of Cincinnati [Center for Business Analytics](#). Prof. Mike Fry discusses [Data Analytics for the Center](#).

Thrust IV. Synthetic Skin, Biomedical Testing Applications



Emergence of hierarchy for biomimetic materials.

What is needed to form CHEM?

Need 9 to 12 members @ ~\$65,000/yr for NSF funding
Need a science/precompetitive approach
For August 30 need a letter of commitment (next slide)
(NSF decision March 2021; Corporate decision
and funding May–June 2021)



We hope to grow to ~30 corporate members in 4 years

Fund research projects targeting pre-competitive industrial needs

Recruit new faculty in this area

Purchase equipment for the center needs

Host topical meetings and workshops

Interchange students with industry

Encourage industrial participation in research projects

Fund industrial residencies for students/post docs (Funded by NSF INTERN)

Host industrial scientists and engineers at the universities

Interact with parallel centers in Europe and Asia

Provide a long-term relationship with potential new hires

For August 30 need a letter of commitment

Required Text:

Should The Center for Emergent Hierarchical Materials (CHEM) be selected by NSF for funding, {Company Name} commits to joining CHEM as a full member at the membership level of \$65,000 on an annual basis, pending availability of funds, and pending acceptance of the NSF's required Membership Agreement.

Participants in this planning meeting:

NIOSH (Centers for Disease Control)

Air Force Research Labs

W. L. Gore & Associates

Procter & Gamble

Dupont

Avery Dennison

Becton Dickenson

Sun Chemical

Michelman

Merck

Shepherd Color

LyondellBasell

Chemours

Sherwin Williams

Bridgestone Firestone

International Paper

Ford

Polyone

ExxonMobil

Omya

Krauss-Maffie

PPG silica

Sumitomo Rubber

Others:

Solvay

Merck

Mirexus Biotechnologies

Heraeus Medical Components

Momentive

Arlanxco

Cabot

AkzoNobel

BASF

SABIC

Novartis

Evonik

Unilever

Colgate

HP

Clariant

Wacker Chemie

Dow Silicones

Nova Chemicals

Ashland Chemicals

3M

Ticona-Celene

IBM

Intel

Johnson & Johnson



Figure 3

Organizational Chart for the Center for Hierarchical Emergent Materials (CHEM)

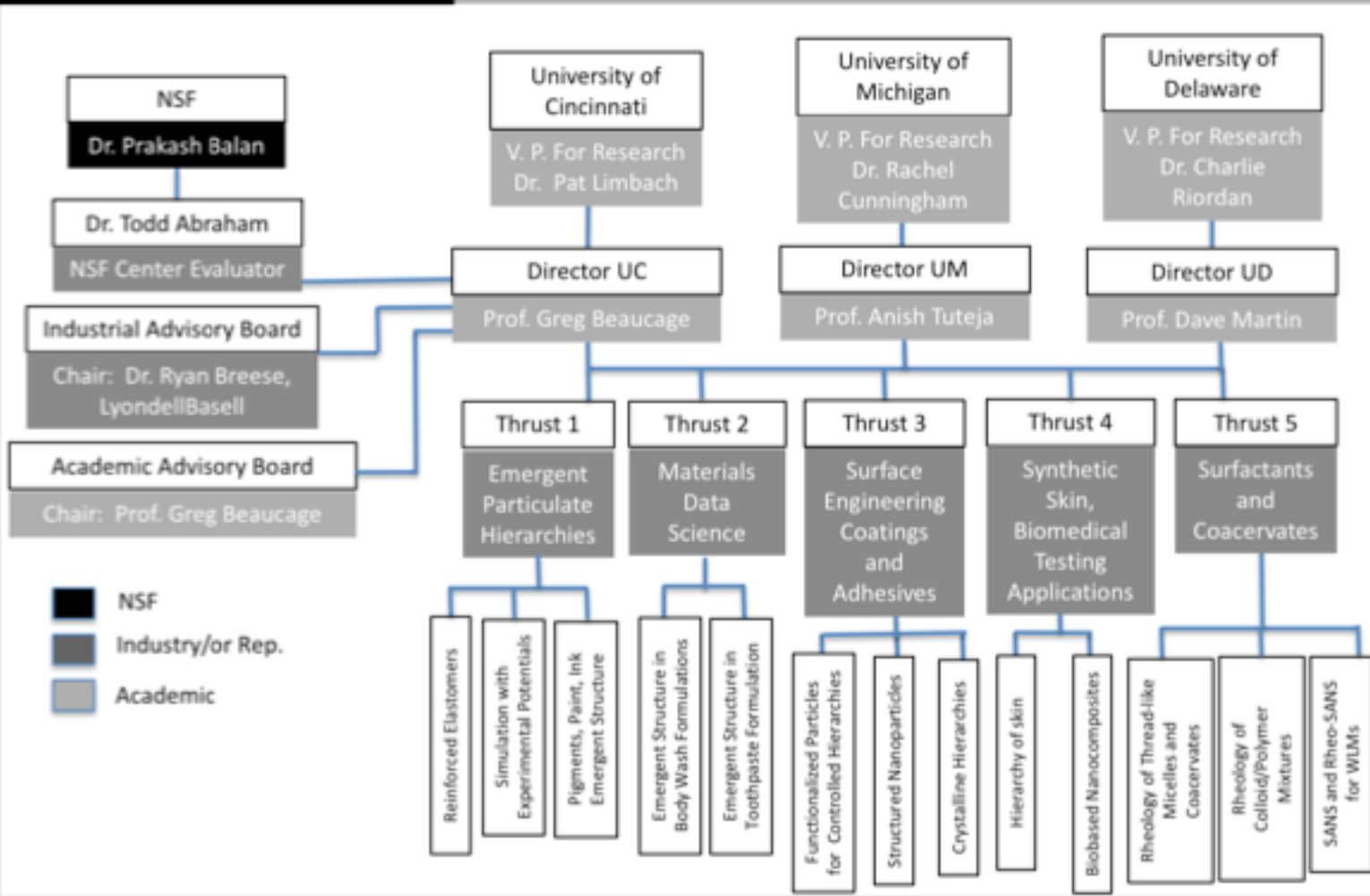
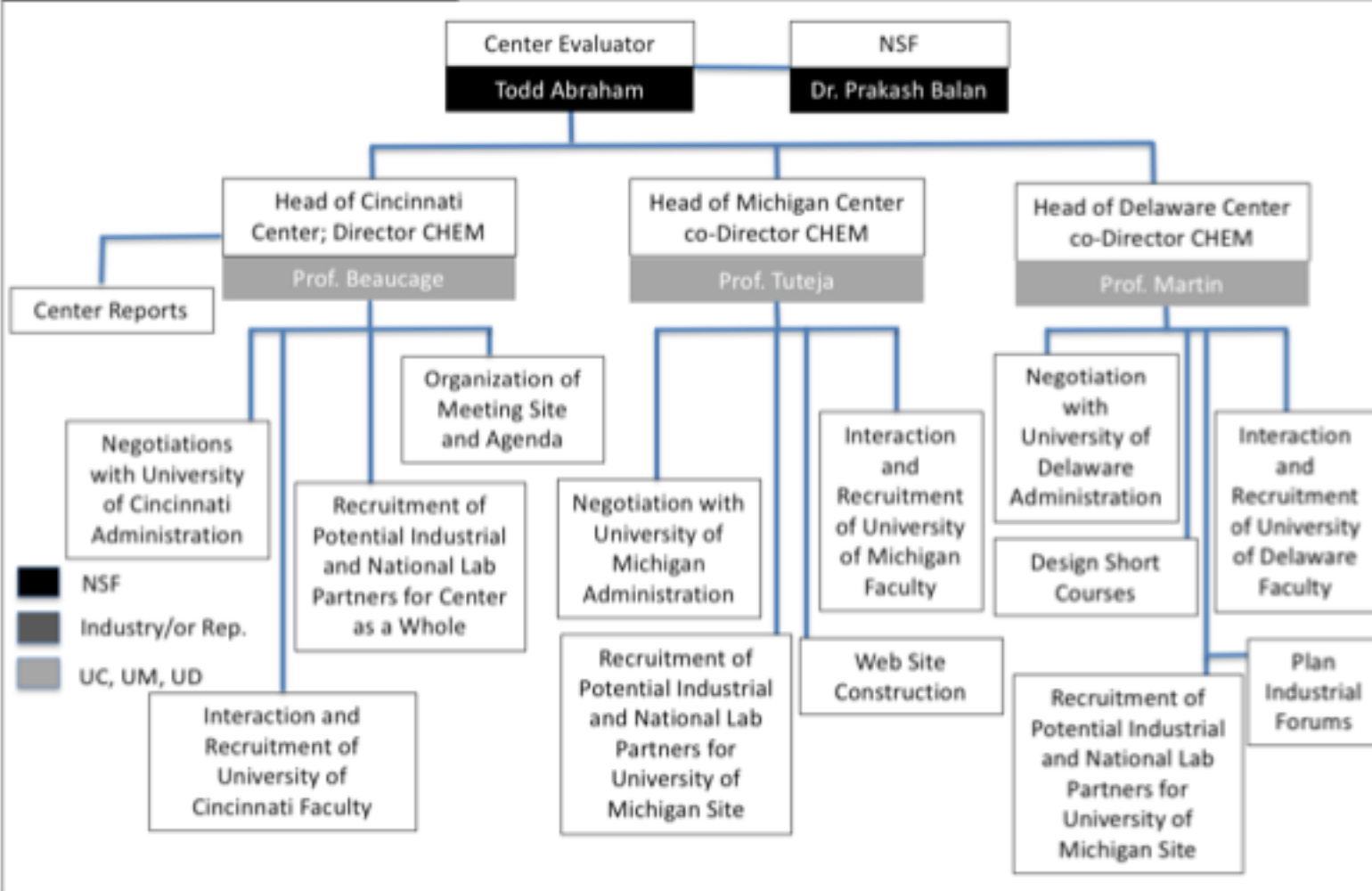


Figure A

Responsibility Matrix The Center for Hierarchical Emergent Materials (CHEM)

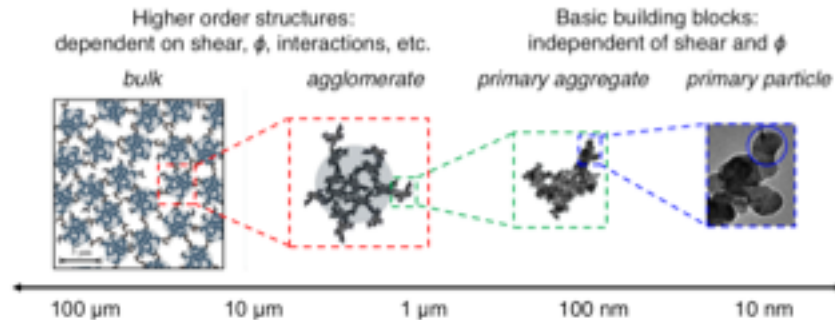


The Center for Hierarchical Emergent Materials (CHEM)



Greg Beaucage, Scattering,
Nanocomposites,
Pigments
Yoonjee Park, Skin/Surfactants,
Biomed delivery
Jon Nickels, Scattering,
Aqueous Systems
Neil Ayers, Synthesis,
Polymers,
Surfactants,
Surfaces

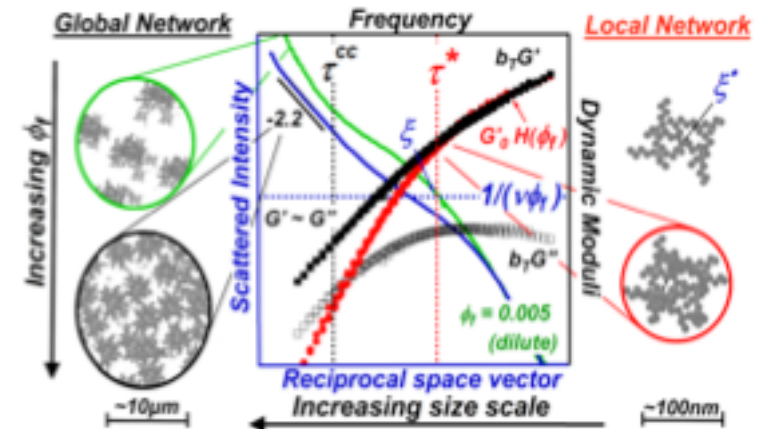
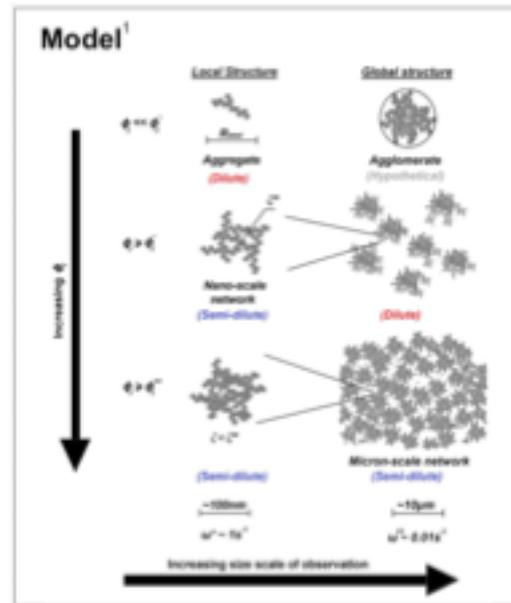
Tires



Batteries

Julie Hipp, Jeffery Richards, Norm Wagner (2017 & 2019 **Poster 001**) Cabot/AkzoNobel

Kabir Rishi, Greg Beaucage (2018
Poster 002) Bridgestone



The Center for Hierarchical Emergent Materials (CHEM)

Hierarchy of Skin in the Presence of Surfactants and Moisturizers

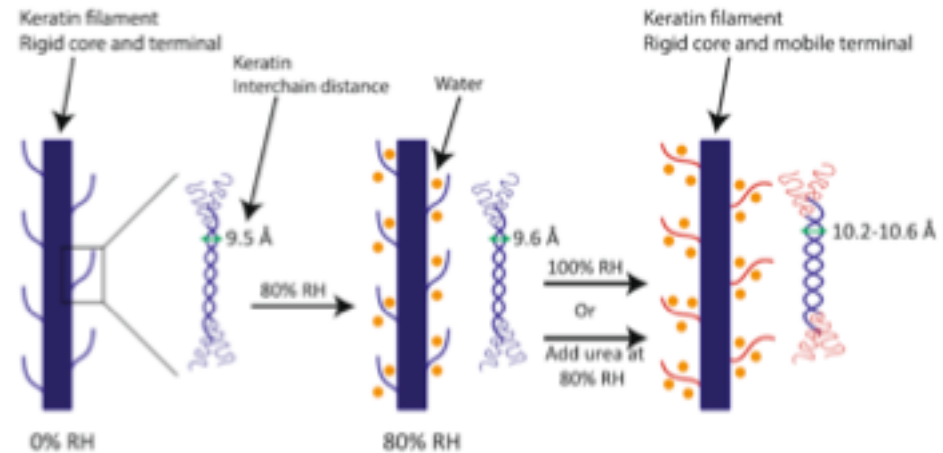


Greg Beaucage, Scattering,
Nanocomposites,
Pigments

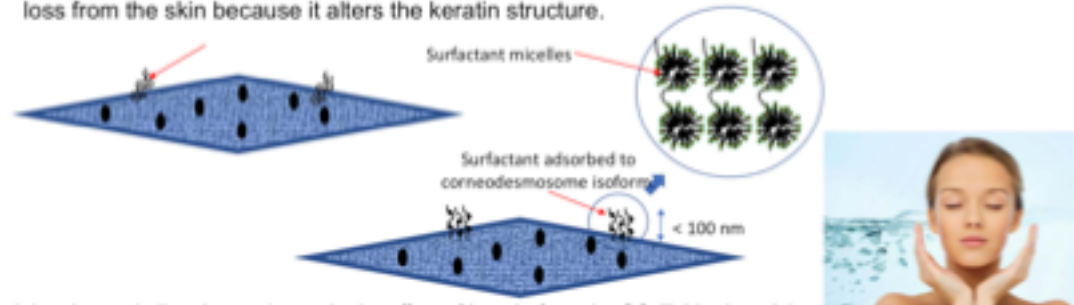
Yoonjee Park,
Skin/Surfactants,
Biomed delivery

Jon Nickels, Scattering,
Aqueous Systems

Neil Ayers, Synthesis,
Polymers,
Surfactants,
Surfaces



➤ We hypothesize that surfactant adsorbs on SC, especially keratin filaments, and accelerates water loss from the skin because it alters the keratin structure.



➤ It has been challenging to decouple the effect of keratin from the SC (lipid + keratin).

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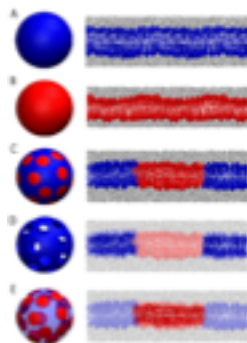


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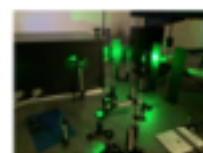
Neil Ayers, Synthesis,
Polymers,
Surfactants,
Surfaces



Isolatic Scattering / Dynamics
Direct / Backscattering / Neutron Spin Echo



Linear Scattering / Structure
SANS/SAXS



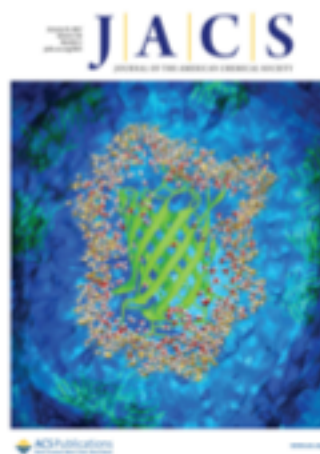
Isolatic Light Scattering



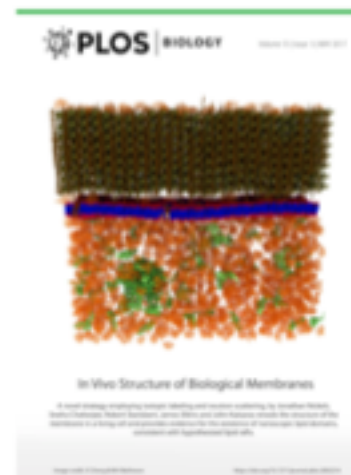
Fluorescence / FRET / Polarization



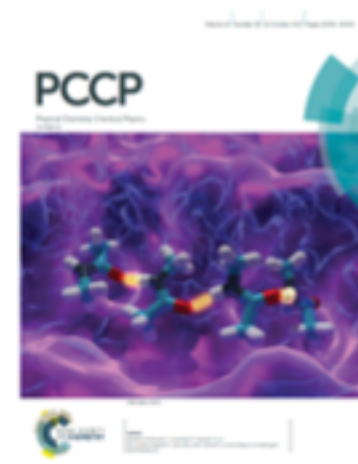
GPU Accelerated
Small S



Hydration water: water
molecules at the interface



Understanding the structure
of biological membranes



Molecular origins of physical
properties in liquids

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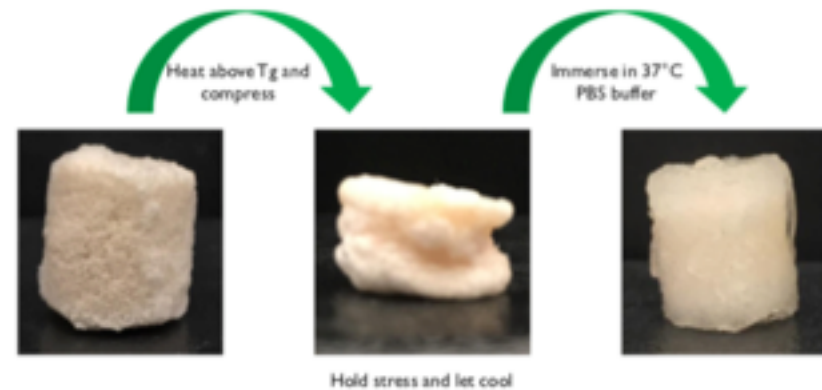
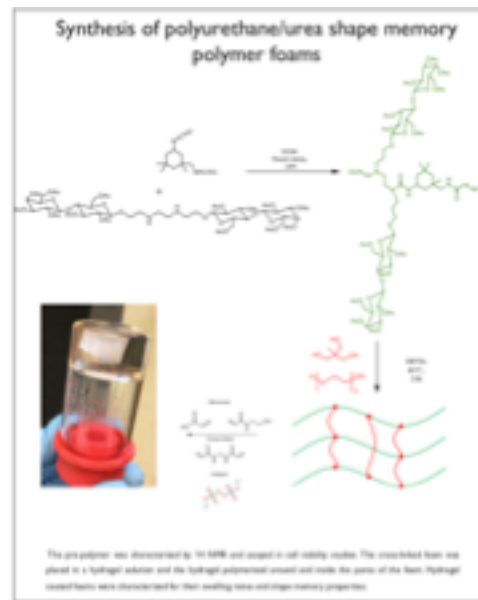
Greg Beaucage, Scattering,
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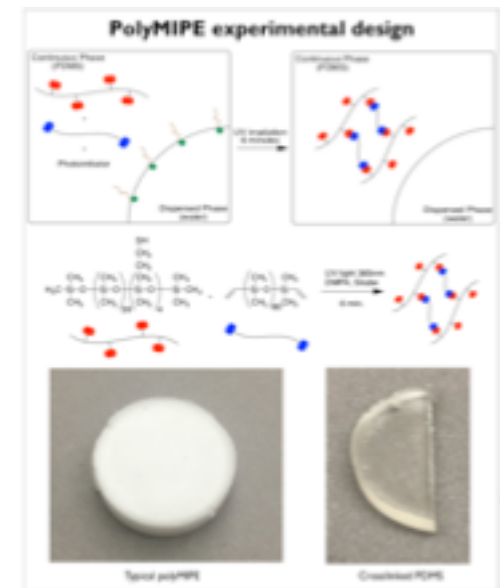
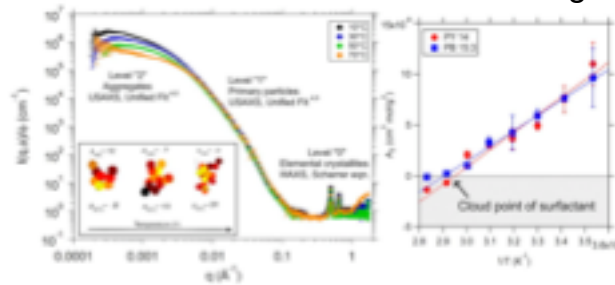
Jon Nickels, Scattering,
Aqueous Systems

Neil Ayers, Synthesis,

Polymers,
Surfactants,
Surfaces



Thermal Control of Emergent
Multi-hierarchical Structure in Commercial Pigments



The Center for Hierarchical Emergent Materials (CHEM)



University of CINCINNATI

AMCC

CONTACT: Melodie Fickenscher, PhD
513-554-3320
fickenem@uc.edu

Scanning Electron Microscopy

- FEI Apreo-C LowVac
- FEI S480 Dual-Beam SEM/TEM

Capabilities

- Low Vac Imaging of non-conductive samples
- Sectioning with Focused Ion Beam
- Elemental Analysis (EDX)
- EBSD
- E-beam Lithography
- STEM

Other Instrumentation

- IRD
- DSC/TGA
- AFM
- TSM
- DLS



Differential Scanning Calorimeter

- MCR 301
- Auto-Tank
- TGA available in private lab



Transmission Electron Microscopy

- CM-100000-LAB
- Elemental Analysis



Atomic Force Microscopy

- Dimension 3100
- Multi-Cell
- Control/Mapping



X-Ray Diffraction

- Panalytical XRD
- XRD-PRO in Research
- XRD software



Light Microscopy

- Zeiss Nikon
- Brightfield/Inverted
- Polarizer
- Reflectance Light
- MicroProjector
- Image Acquisition System

Center for Chemical Sensors & Biosensors

Raman Microscope (Renishaw InVia)
Laser lines: 785, 514, 488, 457 & 442 nm

Nicolet 6700 FT-IR Spectrometer & Microscope

Cary Eclipse Fluorescence Spectrometer

Cary UVVis Absorbance Spectrometer

Philips XL30 Environmental Scanning Electron Microscope



Variable Angle Spectroscopic Ellipsometer

MicroCal Isothermal Titration Calorimeter

Netsch STA 409 PC Simultaneous TGA & DSC

Bio Tek, Synergy 4 Multiplate Reader

Veeco Scanning Probe Microscope
AFM, STM, EFM, MFM

Keyence VHX-1000E Digital Light Microscope

Nuclear Magnetic Resonance Spectrometry

Bruker AVANCE NEO-400
Z-Grad BBFO ATM probe: ^1H , ^{13}C , ^{31}P , ^{15}N
Variable temperature capability

Bruker AV-400
Z-Grad BBFO ATM probe: ^1H , ^{13}C , ^{31}P , ^{15}N
Automatic sample changer
Variable temperature capability

Bruker DMX-500
Z-Grad $^1\text{H}/^{13}\text{C}/^{15}\text{N}$ TXI probe: triple-resonance
Z-Grad BBI probe: ^1H , ^{31}P , ^{15}N
Variable temperature capability



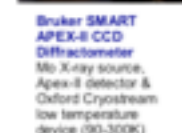
^1H , ^{13}C & multi-nuclear NMR in one and two dimensions including DEPT, 2D ^1H - ^1H COSY & NOESY, 2D ^1H - ^{13}C HSQC and self-diffusion measurements

^1H , ^{13}C and ^{15}N triple resonance in three dimensions for protein structures in solution

Single Crystal X-ray Crystallography



Bruker VENTURE D8 Diffractometer
Mo & Cu microfocus X-ray sources, Photon-II detector & Oxford Cryostream low temperature device (90-500K)



Bruker SMART APEX-III CCD Diffractometer
Mo X-ray source, Apex-II detector & Oxford Cryostream low temperature device (90-300K)



Cambridge Structural Database, Apex3, Shelxt, Clex2, Diamond & other chemical crystallography resources

Synchrotron Radiation via SCrALS at ALS

Stereomicroscopes by Olympus with video & polarizing capability



Thrust II Materials Data Analytics in Coordination with Dr. Mike Fry of UC Center for Business Analytics (Section C of the program Analytic Centers)

The central diagram illustrates the Center for Business Analytics ecosystem, with five interconnected red circles: **Students** (top), **Faculty** (bottom), **Analysts** (left), **Analytic Leaders** (right), and **Center for Business Analytics** (center). The entire diagram is set against a large, faint red circular background.

Surrounding the diagram are four video thumbnails:

- Member Forums:** A video titled "Fry CHEM Intro" showing a group of people in a meeting room.
- Public Education:** A video titled "ANALYTICS SUMMIT 2018" featuring a speaker and a building.
- Student Projects:** A video showing a group of students in red shirts posing for a photo.
- Public Training Courses:** A video showcasing logos for various data science tools: R, Python, Tableau, Hadoop, Excel, Power BI, and Spark.

Anish Tuteja, Site Director Michigan
Dave Martin, Site Director Delaware

NSF: Barbara Ransom, Program Manager
NSF: Todd Abraham, Center Evaluator and L.I.F.E. forms

15 minute break

Section B: Breakouts with Faculty
(Kabir Rishi: rishikr@mail.uc.edu, 513 888-1879)

Lunch

Section C: Breakouts with Analytic Facilities and Data Analytics
Section D: Industrial Mixer
Closing Remarks

Dinner

Section E: Posters



The meeting is an information gathering exercise for companies to understand what the Center could offer but also for the PIs so we can formulate a relevant Center that provides value