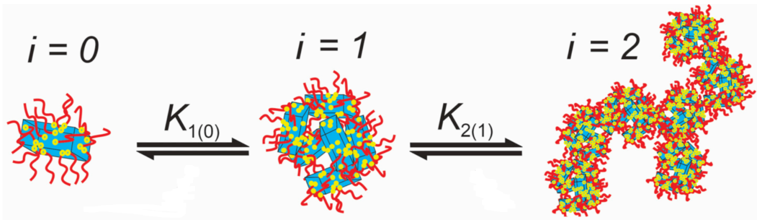
The Center for Hierarchical Emergent Materials (CHEM)

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, coacerverates, biomimetic and biological systems.

SHERWIN WILLIAMS®

The Center for Hierarchical Emergent Materials (CHEM)

University of Cincinnati

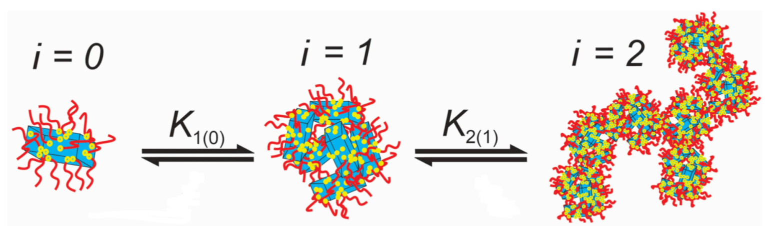
Greg Beaucage, Scattering, Nanocomposites, Pigments
Yoonjee Park, Skin/Surfactants, Biomed delivery
Jon Nickels, Scattering, Aqueous Systems
Neil Ayers, Synthesis, Polymers, Surfactants, Surfaces

University of Delaware

Dave Martin, Microscopy, Conjugated Polymers, Crystalline Structure
Arthi Jayaraman, Simulation, Polymer Grafted Nanoparticles
Darrin Pochan, Surfactants, Polymers, Microscopy
Norm Wagner, Rheology, Scattering

University of Michigan

Anish Tuteja, Surfaces, Dispersion
Nick Kotov, Complex Hierarchies
Ron Larson, Rheology, Simulation
Jinsang Kim, Synthesis, Polymers, Biomedical, Sensors



The Center for Hierarchical Emergent Materials (CHEM)

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 II. Materials Data Science

This thrust involves develoment of tools to utlize large data sets towards targeted goals involving formulation chemistry targeting hierarchical emergence. This Thrust will be in collaboraton with the University of Cincinnati Center for Business Analytics. Prof. Mike Fry discusses Data Analytics for the Center.

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 IV. Synthetic Skin, Biomedical Testing Applications

Emergence of hierarchy for biomimetic materials.

Thrust V. Surfactants and Coacervates

Emergent hierarchical structures in surfactant systems.

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:

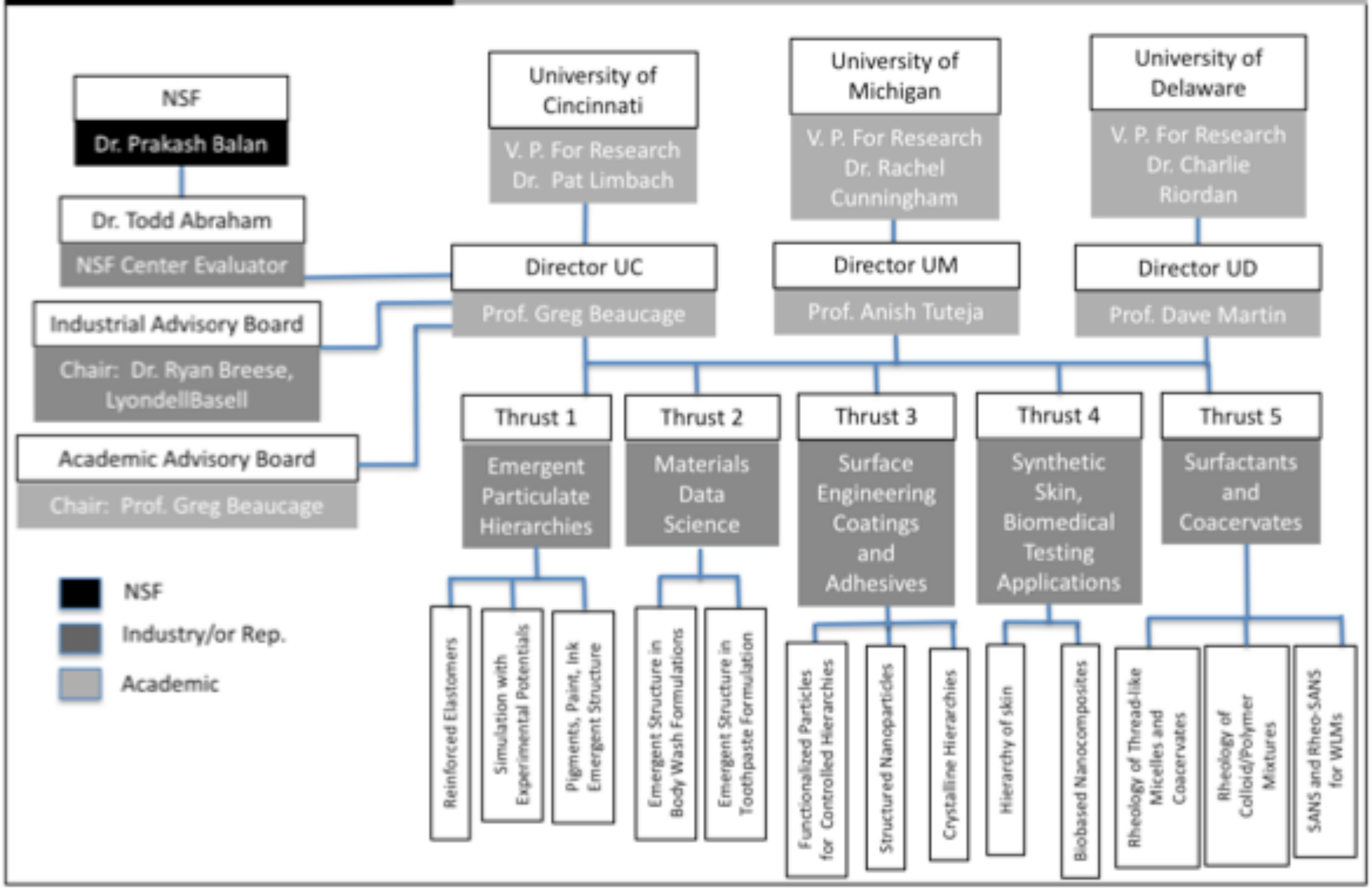
NIOSH (Centers for Disease Control)
Air Force Research Labs
W. L. Gore & Associates
Procter & Gamble
Dupont
Avery Dennison
Becton Dickenson
Sun Chemical
Michelman
Merck
Shepherd Color
LyondellBasell
Chemours
Sherwin Williams
Bridgestone Firestone
International Paper
Ford
Polyone
ExxonMobil
Omya
Krauss-Maffie
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-Celenese
IBM
Intel
Johnson & Johnson

Figure 3 Organizational Chart for the Center for Center for Hierarchical Emergent Materials (*CHEM*)



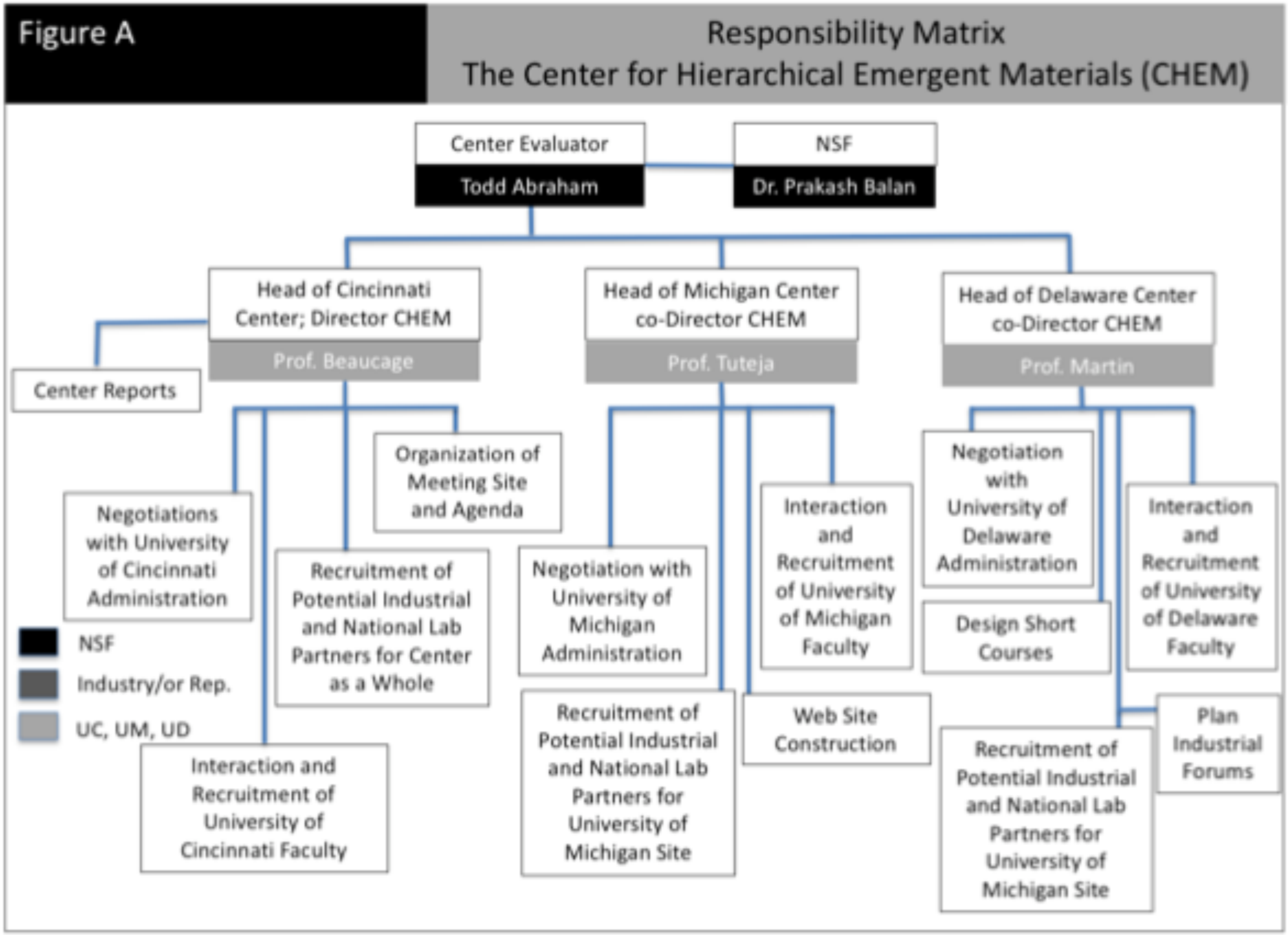


Figure A
Responsibility Matrix
The Center for Hierarchical Emergent Materials (CHEM)
Center Evaluator
Todd Abraham
NSF
Dr. Prakash Balan
Head of Cincinnati Center; Director CHEM
Prof. Beaucage
Head of Michigan Center co-Director CHEM
Prof. Tuteja
Head of Delaware Center co-Director CHEM
Prof. Martin
Center Reports
Organization of Meeting Site and Agenda
Negotiations with University of Cincinnati Administration
Recruitment of Potential Industrial and National Lab Partners for Center as a Whole
Interaction and Recruitment of University of Cincinnati Faculty
Negotiation with University of Michigan Administration
Interaction and Recruitment of University of Michigan Faculty
Recruitment of Potential Industrial and National Lab Partners for University of Michigan Site
Web Site Construction
Negotiation with University of Delaware Administration
Design Short Courses
Interaction and Recruitment of University of Delaware Faculty
Plan Industrial Forums
Recruitment of Potential Industrial and National Lab Partners for University of Michigan Site
NSF
Industry/or Rep.
UC, UM, UD

The Center for Hierarchical Emergent Materials (CHEM)

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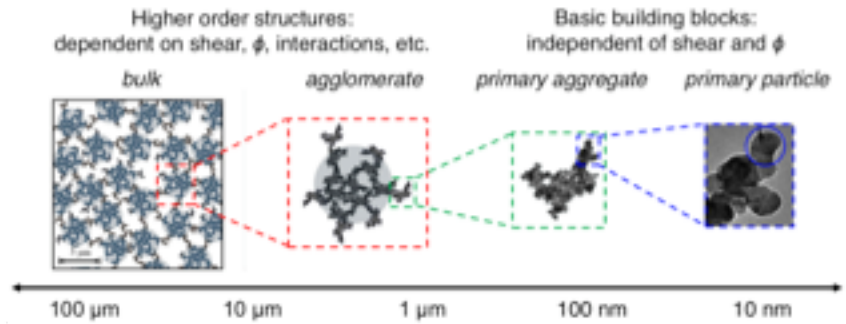
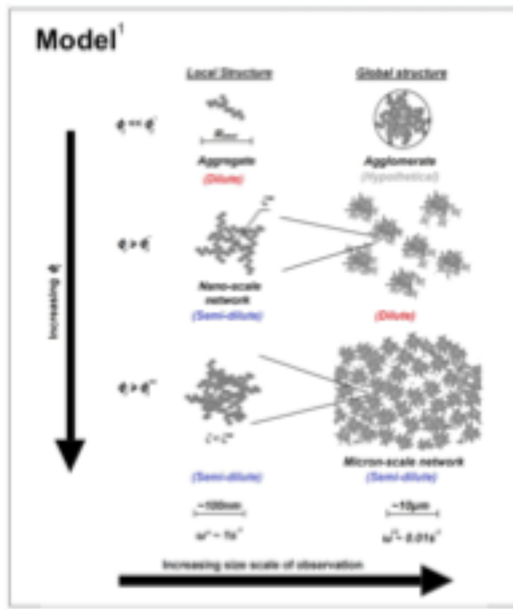


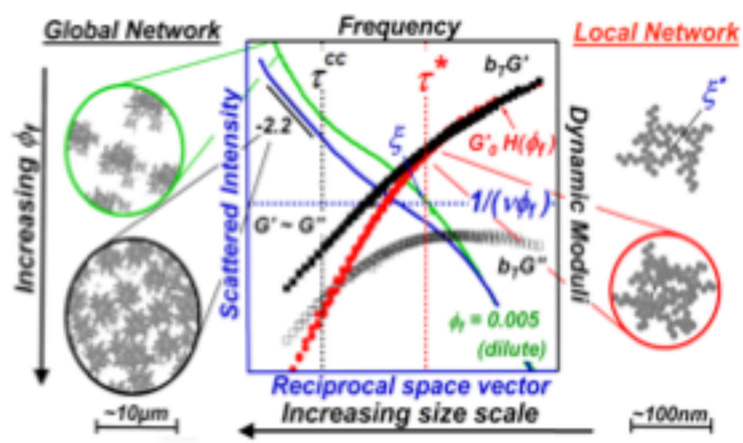
Batteries

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

Tires



Kabir Rishi, Greg Beaucage (2018 **Poster 002**) Bridgestone



The Center for Hierarchical Emergent Materials (CHEM)

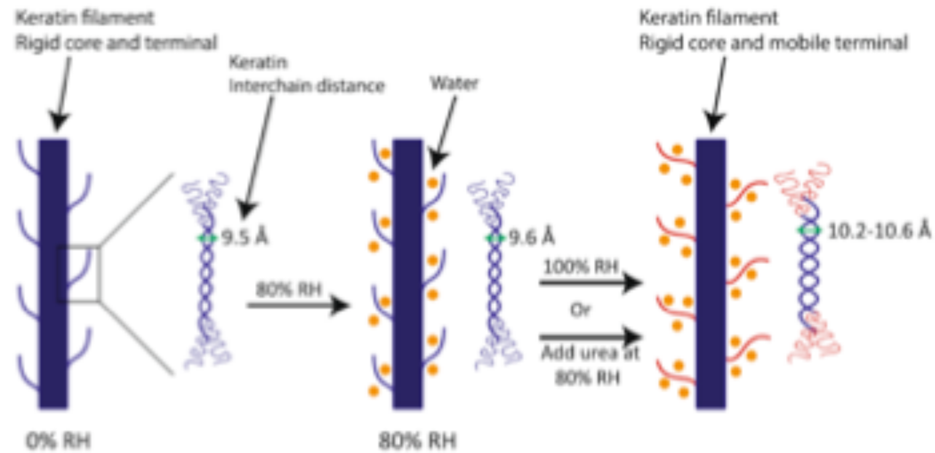
Hierarchy of Skin in the Presence of Surfactants and Moisturizers

Greg Beaucage, Scattering, Nanocomposites, Pigments

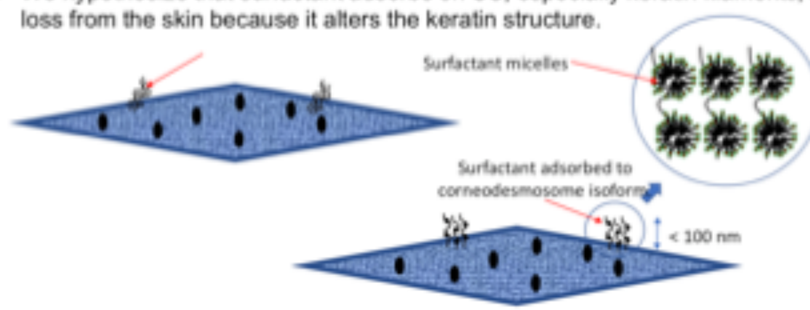
Yoonjee Park, Skin/Surfactants, Biomed delivery

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).

The Center for Hierarchical Emergent Materials (CHEM)

University of Cincinnati

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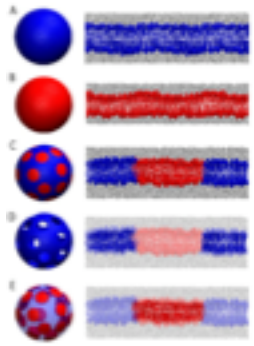
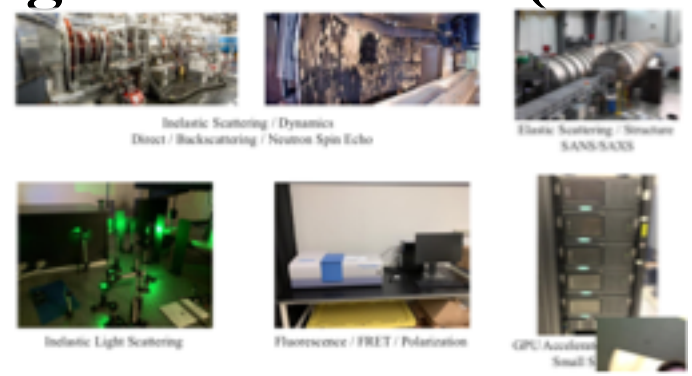
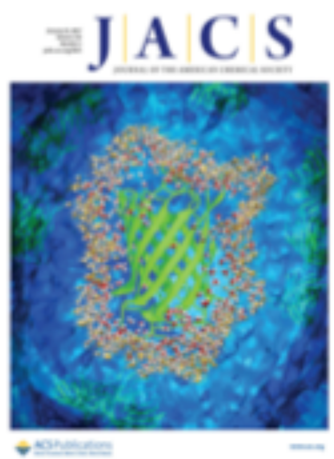
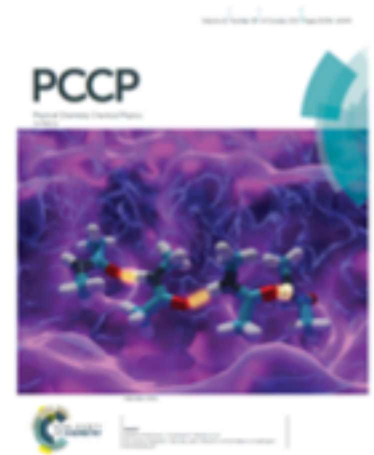






Hydration water: water molecules at the interface

Understanding the structure of biological membranes



Molecular origins of physical properties in liquids

The Center for Hierarchical Emergent Materials (CHEM)

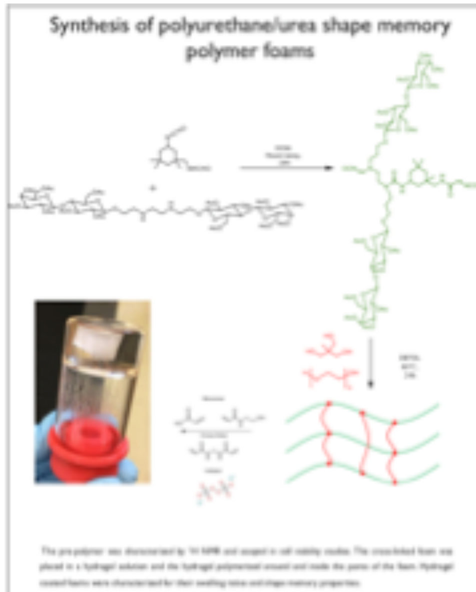
University of CINCINNATI

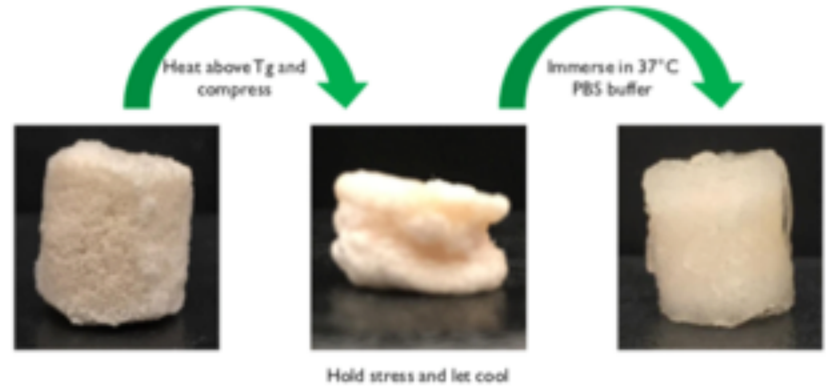
Greg Beaucage, Scattering, Nanocomposites, Pigments

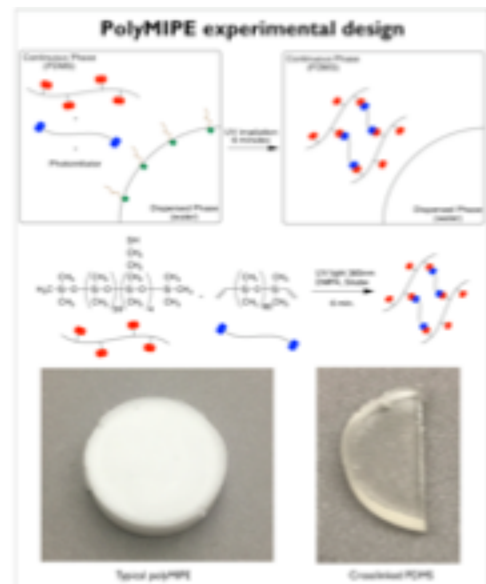
Yoonjee Park, Skin/Surfactants, Biomed delivery

Jon Nickels, Scattering, Aqueous Systems

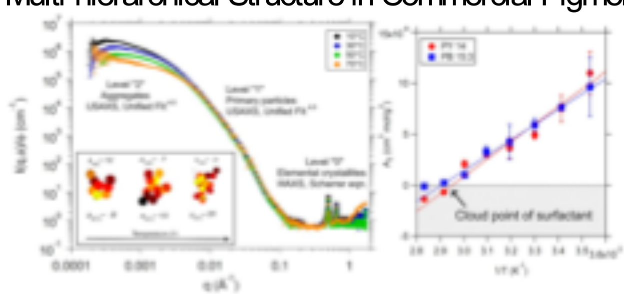
Neil Ayers, Synthesis, Polymers, Surfactants, Surfaces





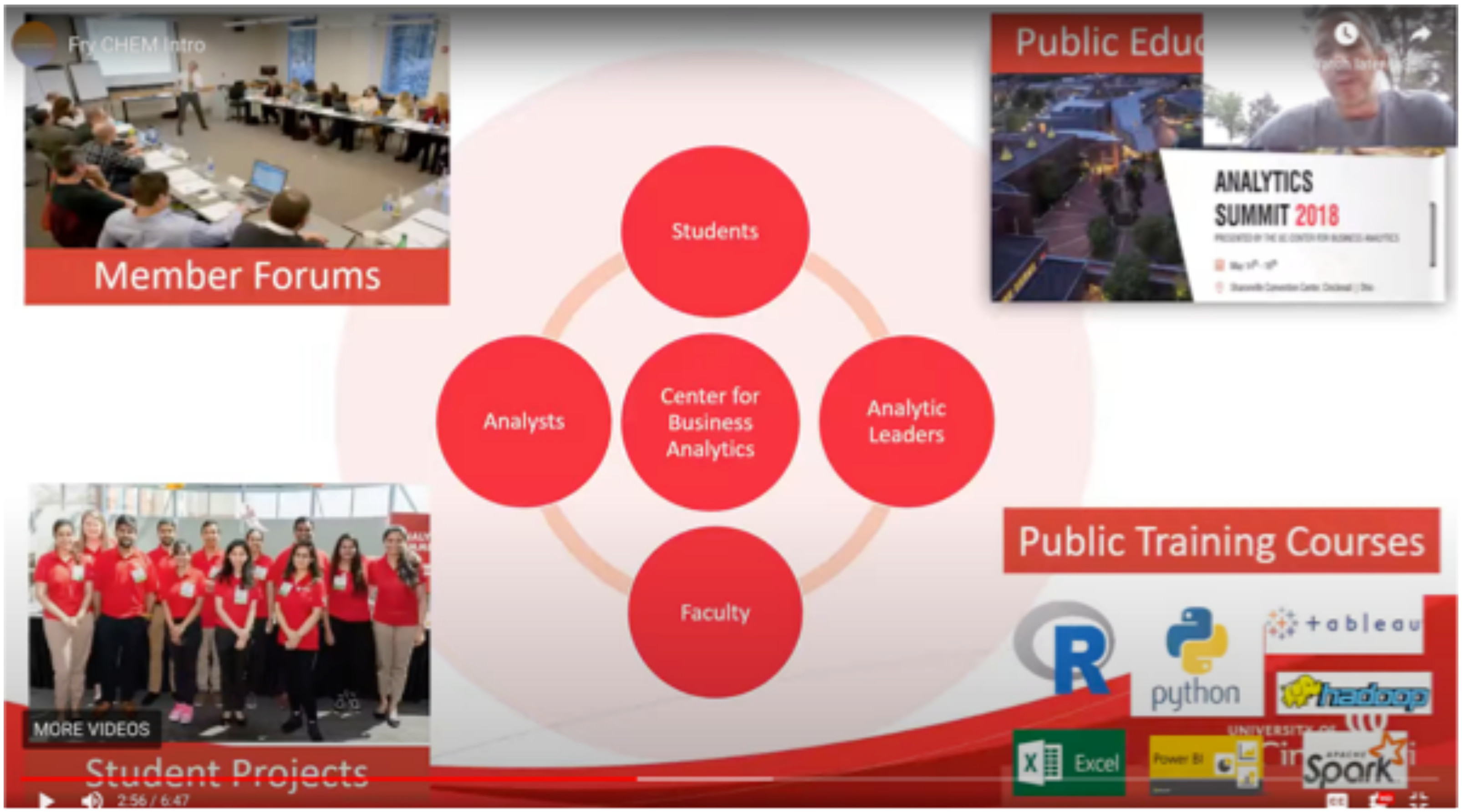


Thermal Control of Emergent
Multi-hierarchical Structure in Commercial Pigments



The Center for Hierarchical Emergent Materials (CHEM)

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



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