PROJECT SUMMARY

Overview:

A gap exists between lab-scale research of nanoparticle, colloidal and biomimetic systems and their commercial application. One part of this gap is that lab-based systems tend to show miscibility and be limited to a single structural feature such as packing of colloidal spheres into a colloidal crystal. The latter is an example of a material with a single structural and dynamic level. Many commercial materials display several structural or dynamic levels associated with different length scales, frequency scales, optical absorption or scattering scales, biological relevance scales and the like. These are more complex, multi-hierarchical materials composed of hierarchies upon hierarchies. An example is the filler network in a tire composed of primary nanoparticles which aggregate, then cluster into a nano-network which itself percolates to form a macroscopic network. In this case the structure emerges serendipitously from processing conditions mitigated by the surface area and interfacial interactions. Different parts of the structure impact different aspects of the dynamic response, the nano-network impacting highway speeds, the micron-scale network impacting tear resistance and low speed robustness. Often the multi-hierarchies have time dependence to their structural maturation and performance, i.e. "4D materials". This is the case as an ink dries on paper developing a multi-hierarchical structure that interacts with light. The Center for Hierarchical Emergent Materials (CHEM) assembles a team of twelve world leaders in research from three universities, Michigan, Cincinnati and Delaware, to find synergy in their efforts to understand, design, and control these complex commercial materials.

Intellectual Merit:

The Center will have direct impact on products such as biomedical devices, shampoo, tires, inkjet inks, rapid prototyping materials, filtration media, catalyst supports, paints and cosmetics and skin care products. Synergy is expected by comparing advances between divergent fields and by interactions between researchers focusing in the fundamental aspects of emergent hierarchies. The Center will add to our understanding of the assembly of complex multi-hierarchies leading to computational and experimental tools that will enable new technology in these areas, shedding light on a largely empirical and serendipitous area of technology and science.

Broader Impacts:

CHEM will develop human capacity in the chemical processing, and consumer products industry by training new PhD, MS and BS scientists and educating industrial practitioners. The center will significantly enhance the nation's research infrastructure base. This is a unique initiative that places the US scientific community at the front of area obviously requiring investment for the manufacture of complex hierarchical materials. The center will coordinate internet-based video courses on rheology, scattering, synthesis, microscopy, simulation, and modeling of complex hierarchically emergent systems that will be available to industrial as well as academic participants and the general public on arrangement with the Universities. Short courses will be offered by CHEM. The Center will actively recruit women and minority graduate and undergraduate students. A REU program focusing on minorities, the handicapped, and women will be associated with the Center with students crossing the three campuses for research work. The center offers the unique education experience of working in a multi-campus team partnering with many well-known as well as small-scale industrial partners and national laboratories. The center has as a main goal enhancement of the intellectual capacity of the engineering workforce and capabilities in controlling emergent hierarchical materials. Improvement in our control of these complex structures will lead directly to improvements in a wide range of consumer and industrial products from hair gels to conveyor belts; from sutures to viscosity enhancers.

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Appendix Items:

*Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

Planning Grant Objective

Objective: The objective of this planning grant is to organize and plan the Center for Hierarchical Emergent Materials (CHEM). The grant will support a meeting organized by the Academic PI's from the Universities of Michigan, Delaware, and Cincinnati with potential industrial, military and national laboratory partners and other interested parties such as representatives of the university administrations and the Center Evaluator. This meeting will be used to determine the initial research agenda, organization and types of memberships/affiliations in the Center.

Strategy: The CHEM will be developed in collaboration with the academic PI's, university administrators, industrial partners, NSF representatives, and the Evaluator. Much of the center planning will take place at the Planning Meeting in the fall of 2019 at the University of Cincinnati. The strategy for implementing the objectives will be to present a proposed format for the center and several other optional formats as proposed by industrial and national lab participants. The Centers academic PI's will use inputs from the planning meeting to mold the Center organization to match the interests of those financially supporting the Center as well as the academic interests of the Universities.

Potential Members:

Letter Attached (20)

Solvay
W. L. Gore & Associates
Procter & Gamble (Diaper Division)
Merck
Sumitomo Rubber Industries
The Chemours Company
The Shepherd Color Company
Mirexus Biotechnologies Inc.
Avery Dennison
Sun Chemical
Procter & Gamble (Corporate Functions R&D)
Bridgestone Americas Inc.
Air Force Research Laboratory (Emergent Materials)
Dupont, Biomaterial
Oak Ridge National Laboratory
Argonne National Laboratory
Air Force Research Laboratory (Structural Materials Division, Composites Branch)
PPG
Omya Inc.
Heraeus Medical Components, LLC

Expecting Letter (e-mail confirmation 9)

Dow Chemical
Procter & Gamble (Beauty and Skincare Division)
LyondellBasell
Polyone
ExxonMobil
Momentive
Arlanxco
Ford
Moderna

Awaiting Reply (11)

Goodyear Tire and Rubber
Sherwin Williams
BASF
SABIC Americas
KaoCollins
Michaelman
Continental Tire
Michelin
Novartis
Evonik
Unilever
HP
Clariant
Celanese
Wacker Chemie
Dow Silicones
Goodrich Tire
Nova Chemicals
Ashland Chemicals
3M
Tocona Corporation
IBM
Intel
Johnson & Johnson

Meeting Planning:

Location: University of Cincinnati, Kingsgate Conference Center

Tentative Date: October, 2019

Meeting Format and Organization: A draft agenda for the planning meeting is shown in the Supplemental Documents Section. The meeting will open with brief remarks from the Vice President for Research at the University of Cincinnati and from administrative representatives of the Universities of Michigan and Delaware. These speakers will be introduced by the three PI's. The introductory remarks will be followed by a description of the vision for the center and the benefits center membership will have for the participating center members. The NSF program director (or other representative of NSF) will next present a description of the I/UCRC program and NSF's expectations for the Center. The Center Evaluator will be introduced and will give a few remarks on his/her role and interaction with the Center. This will be followed, after a short break, by presentation of several proposed research projects for Thrust 1. After Lunch, projects from Thrusts 2 and 3 will be described. A booklet with one-page descriptions of possible projects form the three universities will be provided. The attendees will also be forwarded a form to suggest projects prior to the meeting and these will be included in the CMT booklet. For both Project Presentation sessions LIFE (level of interest, feedback & evaluation) evaluation forms or computer forms will be distributed and collected giving feedback on the proposed projects. In the late afternoon a session that invites input for proposed projects from the industrial participants will be held. Discussion of industrial and national lab input will also be sought during a social hour with project proposal posters in the evening. Meeting participants will be on their own for dinner.

In the second day there will be an industry-moderated session with moderators selected at the end of the first day during the discussion session. This will be followed by an NSF-moderated session where the LIFE evaluations are summarized and discussed. Finally, the NSF representative will have a closed-door session with the industrial participants to aid in evaluation of the center proposal. The three PI's will close the meeting around noon on the second day.

A summary of the meeting with selected initial research topics and center members will be distributed to the participants a short time after the planning meeting.

Responsibilities of Presenters: The tasks of the meeting participants are listed below:

<u>Prof. Greg Beaucage, Prof. Dave Martin & Prof. Nick Kotov:</u> Organization of the meeting. Co-presentation of the Center vision and site capabilities. Presentation of the proposed initial projects for the Center. Moderate the Industrial Workshop in the first day. Ensure that LIFE forms are filled out, collected and logged for the NSF Representative. Organize and coordinate the poster session and canvas the industrial and national lab participants for new directions for the Center. Organize the Industry Feedback session for the second day by choosing an industrial moderator and providing necessary support for the session.

<u>Center Evaluator:</u> The Center Evaluator will be responsible for assessing the Center planning meeting and for providing advice concerning setup of the Center and operation of the Planning Meeting. The Evaluator should provide written feedback on the Planning Meeting that can be used in developing the Center Proposal.

<u>NSF Representative:</u> The NSF Representative will provide an overview of the I/UCRC program and will indicate how he/she thinks that the proposed Center could mesh with the existing programs and interest of the NSF and the I/UCRC program. On the second day the NSF representative will moderate the LIFE Form review and discussion. The representative will also hold a closed session with the industrial and national lab participants to discuss the viability of

the Center. The NSF representative will provide feedback to the PI's that can be used to modify the Center proposal.

Industrial/National Laboratory Participants: The industrial and national lab participants will attend the project presentations and provide LIFE feedback forms rating the projects presented. They will provide ideas for additional and alternative projects during the industry workshop. One of the industrial or national lab participants will be chosen to moderate the Industrial Workshop on the second day. The participants are also expected to contribute to the discussions on the Center on the second day.

Project Description

General Analysis of Industry:

Manufacture of a wide range of materials from paints to detergents involves control over structure at size scales from the nano to macroscopic and dynamic properties from static to hundreds of hertz during processing and application. Across these many orders of magnitude in size and frequency it is found that distinct hierarchical levels exist related to thermodynamic conditions and kinetic phenomena. For instance, reinforcing fillers display primary particles which determine the specific surface area, aggregates which determine the local density and moderate to high frequency response, and agglomerates of aggregates that can form macroscopic networks related to properties at high extension and low frequency. There is a reasonable understanding of the manufacture of simple single structural level materials based on thermodynamics, computer simulation, experimental verification and industrial experience. For example, the miscibility limit for two polymers can be predicted based on molecular understanding to predict the second virial coefficient or the interaction parameter using PRISM theory, or experimental measurement. Most metals and ceramics are based on a single structural level and can be understood using simple thermodynamic and kinetic models.

Intellectual Merit: Complex, hierarchical, "soft" materials occupy a significant economic sector with a broad range of application from catalyst supports and filtration media to biomedical materials, foods and tires. These materials are based on multilevel hierarchies of structure that cannot be simply predicted from a molecular basis. In this case we consider properties across a spectrum of frequency with distinct regimes or dynamic levels related to structure across four or five orders of size displaying distinct structural levels. The thermodynamics of interaction are predictable within a single hierarchical level based on a fixed interaction potential, but this interaction potential changes at other levels with different dynamic properties and related structural architecture. Properties of commercial products are based on this hierarchically description, for instance it is desirable for shampoo to flow under moderate shear rate, but to maintain a gel structure under low shear rate. These properties should vanish on dilution with rinsing. Similarly, tires should show different properties at high frequencies encountered at highway speeds compared to low frequencies when parked or in city traffic. Printed electronics require hierarchical self-assembly during drying of aggregated conductive nanoparticules which form an emergent macroscopic network related to the final performance. Similarly, the opacity of printed inks and paints depends largely on an emergent macroscopic network tied to the drying process. Industries based on these complex soft materials survive on an understanding of molecular and nanoscale characterization but must use empirical approaches to determine the properties of the final products closely tied to a complex hierarchy controlled by kinetics and thermodynamics. It is the purpose of CHEM to develop tools to understand, predict and control the emergence of these complex multi-hierarchies from relatively simple nano to micro structures such as aqueous dispersions of pigment nanocrystals and surfactants, or synthetic proteins.

The individual academic groups in the proposed Center have each contributed to addressing understanding of the control of complex emergent hierarchical structures and their dynamics. First, since the topic involves processing of complex fluids two Bingham Medal winning rheologists, Ron

Larson and Norm Wagner, have explored polymer, surfactant, nanocomposite systems leading to theoretical, modeling, and experiential advancements. Arthi Jayaraman has used PRISM theory to guide simulations of polymer and nanocomposite systems, Neil Ayres has worked on surface grafting to tune hierarchical growth, Nick Kotov has developed novel nanostructures that could be used to control hierarchical emergence, Greg Beaucage has worked in scattering studies of a myriad of complex hierarchical systems and developed the primary scattering model for such systems, Darrin Pochan is editor of Soft Matter and an expert in surfactant and complex hierarchical systems, Dave Martin is a world leader in TEM and SEM for soft matter hierarchical systems. Jinsang Kim has expertise in synthesis of hierarchical polymers for conductivity and phosphors. Anish Tuteja is an expert in controlled surface compatibility. The center also includes some young faculty with significant industrial links in this area. Jon Nickels is an expert in hydration of biomaterials and has worked with polysaccharide nanoparticle assembly for skin care lotions. Yonjee Park is an expert at biomedical delivery devices using hierarchical structures. A formidable team is assembled that has the skill set to make major advancements on an individual basis and to attract individual industrial support through the center. The center presents an opportunity for synergy across these fields of application and for a cross disciplinary approach. For example, Ron Larson led a project with Procter & Gamble and Greg Beaucage to understand the structural basis for hierarchical rheological response in worm-like micelles. The team links direct measurements of structure using small-angle neutron scattering, simulations of chain structure and rheology measurements to produce a software tool to predict the dynamic rheological response. Darrin Pochan has also contributed to this effort through his expertise in cryo-TEM and the world-class microscopy facilities at the University of Delaware. Norm Wagner has published extensively in this area and could contribute simultaneous in situ SANS, dielectric spectroscopy, and rheology measurements. This type of multi-PI effort can be uniquely assembled and financed through the center. Symbiotic efforts are especially true in coupling simulation work from Arthi Jayaraman's group with experimental measurements. One of Arthi's students, Tyler Martin, is already contributing to the WLM work, though he is now at NIST. Similar collaboration between Jayaraman and the other groups as well as involvement of the synthesis groups in surface modification, growth of complex particles, modification of surface hydrophilicity, with the characterization and modeling expertise, can take full synergistic advantage of the Center.

At the October Center planning meeting, mechanisms for the encouragement of synergistic projects will be discussed. This could include higher ranking for proposals involving multiple research groups or allocation of high funding to support collaborative efforts. Some projects will obviously involve only one group, but it should be clear that interaction through the Center meetings will allow for cross germination of ideas and will generate possibilities of further interactions.

The Center plans to link university, industry, and national lab resources to leverage research efforts, facilities and expertise. For example, polymer nanocomposites are best studied in scattering using a wide scattering vector range instrument (USAXS) that is usually available only at national and international user facilities, particularly at the Advanced Photon Source at Argonne National Laboratory and at the European Synchrotron Research Facility in France. A lab source camera is available through the University of Cincinnati but measurement time is two orders of magnitude longer and the data quality is lower. The University of Delaware has a special arrangement with the National Institute of Standards and Technology for the use of neutron scattering facilities through their Center for Neutron Science. The microscopy center at the University of Delaware is of pivotal importance to much of the Centers work. CHEM includes two world class rheology labs. The Center can also provide training through short courses in techniques used in the research effort as described below.

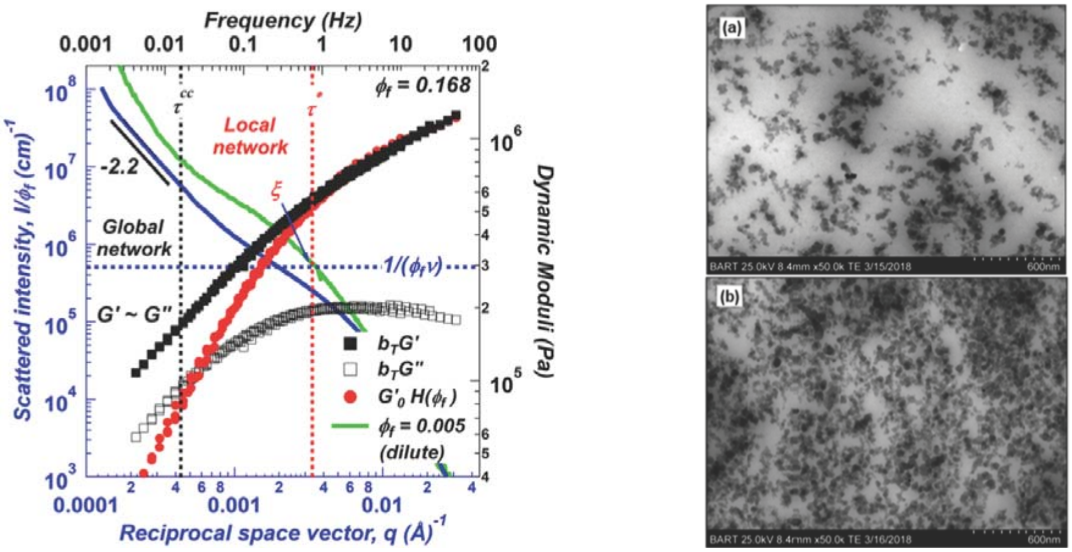


Figure 1. a) Graphical summary of the hierarchical network model as supported by dynamic rheology and structural data. Red circles are for the unfilled elastomer scaled storage modulus. Filled squares are for ϕ_f = 0.168 filled sample storage modulus. Open black squares are the loss modulus for the filled elastomer. The blue line is the scattering curve for the filled sample. Top axis is frequency with dynamic moduli on the right axis; the bottom axis is the reciprocal space vector with the left axis the scattered intensity. Two points link the top and bottom axes, τ to the right (where the scaled neat elastomer diverges from the filled sample, correlating with the nano-network mesh size); and τ_{cc} where gel behavior begins to the left (G' ~ G" ~ ω^p correlating with the macroscopic network scaling regime in scattering) [1]. b) showing dilute (top) and semi-dilute (bottom) conditions. In semi-dilute conditions clusters of aggregates can be seen which percolate to form a micron-size network.*

Existing Capabilities and Expertise:

University of Cincinnati: Greg Beaucage is the Center Lead and the PI for the Cincinnati site. Beaucage's research effort at the University of Cincinnati will involve linking hierarchical structure emerging during processing, application and use to properties [1-10]. There are several areas of interest, elastomer nanocomposites, organic and inorganic pigments, paints and inks, and mass fractal titania and silica for various uses. Beaucage has also worked with worm-like micelle systems with Ron Larson at the University of Michigan (mentioned above). In elastomers Beaucage is interested in linking the dynamic viscoelastic and dielectric response to the hierarchical structure determined with X-ray scattering [1]. An overview of some of Beaucage's work is shown in Figure 1.

Neil Ayres is an expert in chemical modification of surfaces to control interfacial interactions. Work between Beaucage and Ayres will be coupled to tune the emergent hierarchical structure in commercial reinforced elastomers and pigment dispersions.

Yoonjee Park is an Associate Professor in Chemical Engineering who is working on the hierarchical structure of human skin and how it is impacted by skin care products. Procter and Gamble will sponsor this work in the context of the Center. She has previously worked on cardiac drug delivery at MIT and in several other parallel fields.

Jon Nickels is an Assistant Professor in Chemical Engineering with interest in the quantification of bound water in terms of number and strength of association. This is important to the behavior of protein-based drugs, and branched polyscharide nanoparticles used for skin care. Nickels uses elastic and inelastic neutron scattering (SANS, Diffraction, NSE, Backscattering, TOF) among other techniques to quantify these systems. Nickels has attracted a small company, Mirexus, to sponsor this work.

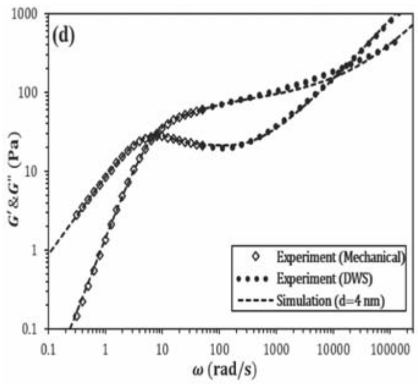
University of Michigan: The PI for the Center at Michigan is Nick Kotov who is well known for his work in biomimetic self-assembly of hierarchical structures, an area in which he has published in *Nature, Science* and *JACS*; and has collaborated with a number of companies including Avery Dennison as well as forming a number of his own companies. His expertise in controlled hierarchical self-assembly of nano-materials as well as his expertise in connecting fundamental research with new products is indispensable to the center. Kotov has collaborated with other members of the center in projects related to hierarchical emergence [11].

Ron Larson is an expert in rheological characterization of polymers and complex fluids. He has pioneered new multi-scale simulation methods for dynamics. Increased computer speeds now allow access to time and length scales relevant for commercially important materials. Larson has made progress in simulations of surfactant-containing shampoos, conditioners, and body washes, latex paints (which include polymers and colloids), and finally, crystallizing polymers. For polyethylene, molecular dynamics simulations and theory are used to describe the effect of short-chain branches and flow on the rate of nucleation of polyethylene crystals and the effect of long-chain branches on rheology. For worm-like micellar solutions, both multi-scale molecular simulations, and micelle-level simulations are used to determine the effect of micelle properties, including length, stiffness, and entanglement density, on rheological properties. Methods of accelerated sampling, including Umbrella Sampling and Forward Flux Sampling, allow information relevant to long time scales to be extracted from molecular simulations. In all cases, emphasis is on knowledge that could lead to commercial impact. An example of a simulation of breakage of a thread-like micelle, to obtain breakage free energy, and of extraction of micelle parameters from fits to rheological data, are shown in Figure 2.

Jinsang Kim is a synthetic chemist with interest in hierarchical materials for biomedical applications. Kim has skill in device creation using phosphorescence, conductivity, to produce biosensors, plastic electronics, and organic phosphors. His expertise in creation of devices will appeal to some participants in the center. Kim has worked extensively with industrial support and has a working relationship with the Air Force Research Laboratory.

Anish Tuteja is an expert in surface modification for improved hydrophobicity and oleopobicity. He has significant industrial support and support from the Air Force Research Laboratory. Tuteja has worked to use his surface modification approaches to tune nanoparticle dispersion which will be advantageous in the Center.

University of Delaware: Dave Martin is the PI for the Center at Delaware. Martin was formerly faculty at Michigan so he serves as a natural link between two sites. He has expertise in high strength polymer fibers which are composed of a crystallographic hierarchy which he has extensively studied with TEM and SEM. Conductive polymers and high strength polymers both display rigid, extended chain structure and Martin has made significant contributions in the study of the crystalline structure of processed conductive polymers. He has recently worked with electrospun polymers. Martin has recruited W. L. Gore, Merck, and others to the Center. Martin has collaborated with Jinsang Kim at Michigan [12].



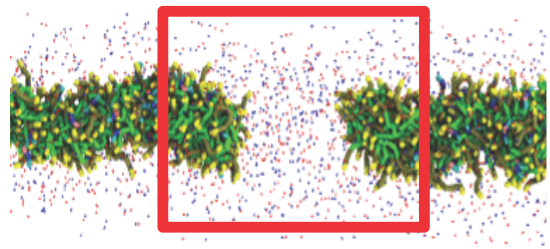


Figure 2 (left) Simulation of breakage of micelle from which the breakage free energy can be extracted using Umbrella Sampling. (right) Experimental measurement of storage (G') and loss (G'') moduli (symbols) of a commercial surfactant solution, fitted by a colloidal scale model (lines), from which micelle length 1.6 µm, persistence length 112 nm, and average micelle breakage time around 0.05 s, can be obtained.

Norm Wagner is a world renowned expert in complex fluid flow as it relates to hierarchical structure. His work covers a broad range of technologies from worm-like micelles to bullet proof armor. Wagner has had extensive interaction with industry. He is head of the Center for Neutron Science at the Unversity of Delaware and is active in the in situ observation of complex fluids under flow, Rheo-SANS, more recenlty coupled with in situ dielectric spectroscopy. Wagner has strong links to many companies such as P&G and DuPont.

Darrin Pochan is the Editor in Chief of Soft Matter and known for innovative research such as entirely biobased nanomaterials and nanocomposites for biomedical and other applications; solution self-assembly; hydrogels; block copolymer nanostructures. Pochan is an expert at cryo-TEM and other microscopy tehcniques as well as neutron and x-ray scattering. Pochan has solicited five companies to the center.

Arthi Jayaraman's group focuses on use of molecular scale features to predict macroscopic structure and thermodynamics using theory and computer simulation. Her contributions involve the use of the PRISM theory and Monte Carlo simulations to predict the evolution of complex hierarchical structure based on interaction potentials. She has recently studied polymer grafted nanoparticle assembly. Jayaraman has links to Dupont, Solvay and Chemours. She will be piviotal as a PI, as well as a collaborator in many areas of research in the center that require modeling and simulation of experimental observations.

Structure of the Center:
Individually, the research groups listed above have made major contribution to the understanding of emergent hierarchical structures in processed materials. The CHEM will provide an enviroment to encourage collaboration between the groups with direction from the industrial advisory board towards targeted goals. Figure 3 shows the structure of the Center.

Diversity Plan:
The CHEM will actively recruit minorities and women to participate in the center research efforts. The center will request REU and RET funding that will specifically target the participation of minority, handicapped, and women undergraduates and high school teachers in the Center's research.

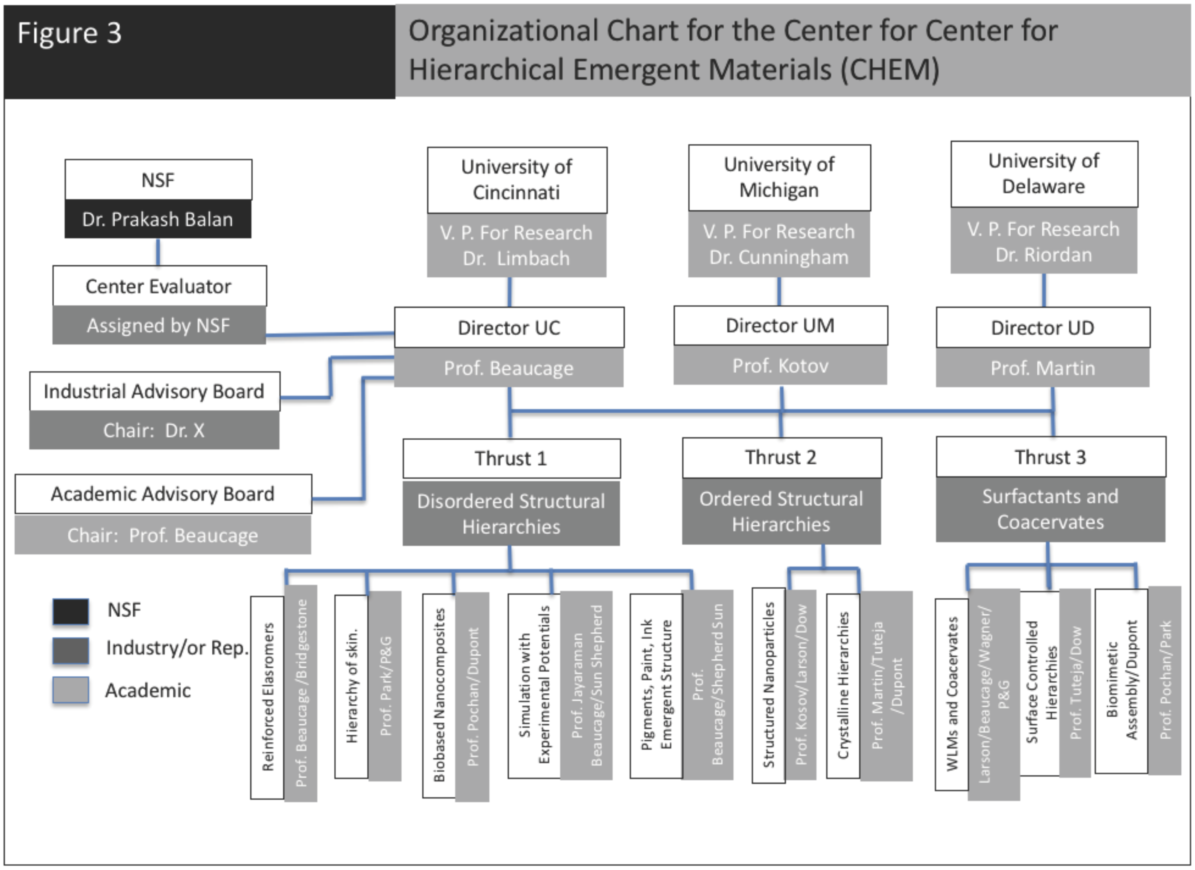


Figure 3 Organizational Chart for the Center for Center for Hierarchical Emergent Materials (CHEM)

Proposed Projects:

A sampling of six of the possible projects that would be pursued by the Center are discussed below to give a flavor of the type of research pursued by the Center. During the planning meeting a large number of specific projects will be discussed in oral presentations and posters. A booklet of one-page project descriptions will be distributed. Industrial participants will be invited to present ideas for projects.

Thrust 1: Disordered Structural Hierarchies

1) Dynamic rheological and dielectric response linked to hierarchical structure and structural emergence for reinforced elastomers.
2) Control of hierarchical structure in skin.
3) Biobased hierarchical nanocomposites.
4) Simulation of emergent macroscopic structure based on experimental nanoscale potentials.

Thrust 2: Ordered Structural Hierarchies

5) Structured nanoparticles for controlled assembly of hierarchies.

Thrust 3: Surfactants and Coacervates

6) Hierarchical dynamics of worm-like micelles and coacervates.

1) Dynamic rheological and dielectric response linked to hierarchical structure and structural emergence for reinforced elastomers.

Proposed Team: G. Beaucage, N. Wagner; Bridgestone, Sumitomo.

Project Objectives: The structure of carbon black and silica in tire compounds can be described by a dual hierarchical network model [1]. Primary particles form aggregates that cluster into nanoscale network domains on milling. Similar behavior is seen in conductive inks on drying, and in conductive fluids for energy applications [16]. These clusters of networks of aggregates percolate above about 20 volume fraction carbon black to form a macroscopic network that has been imaged by X-ray tomography [17]. Moderate to high frequency response from the elastomer compound is controlled by the nano-clusters of aggregates while low frequency and high strain response as well as DC conductivity is related to the macroscopic network of clusters. The project objective is to explore two features of this dynamic response: the time evolution of the dual hierarchical network [18] with aging of milled elastomer compound; and the relationship between emergence and maturation of this complex dual hierarchical network and static and dynamic conductivity as measured in dielectric spectroscopy.

Industrial Relevance: The properties of reinforced elastomers depend on the filler network structure. Control over the network structure could depend on aging effects, the time between filler mixing and elastomer curing. This project will explore the details of this structure property relationship and the links to dynamic conductivity for electronics applications.

Center Relevance: This project directly explores the emergence of hierarchical structures in filled elastomers and their impact on the dynamic viscoelastic and dielectric response.

Experimental Plan: Two types of sample will be prepared, elastomer compounds of carbon black and SBR and polybutadiene rubber, and carbon black in polystyrene. The polystyrene samples will be mixed in a single screw extruder while the rubber samples will be milled in a Braybender mixer. Elastomer samples for rheology and scattering will be prepared and frozen in liquid nitrogen so that the aging time can be determined. The elastomer samples will be warmed to room temperature just before measurement. The glassy polystyrene compounds will be below T_g at room temperature and heated for the measurement. Samples will be aged in the beam and in the rheometer/dielectric spectrometer at temperatures above T_g.

Milestones and Time to Completion: The project will involve biweekly meetings of the project participants to discuss progress using computer conferencing. Organization of X-ray scattering beam time and travel to Argonne National Laboratory for measurements will require approximately 2 months lead time with approximately 3 months for data reduction and analysis. Rheological experiments will follow approximately the same schedule. It is anticipated that the project will run a total of 3 years with the last year focusing on publication of results and completion of experiments after industrial/academic review from the first two years.

Annual and Total Cost to Completion: The project will require a graduate student at the University of Delaware and a graduate student at the University of Cincinnati working in collaboration. The approximate cost per year will be $65,000 per student so a total of $130,000 per year involving two center memberships, total cost of $390,000.

First Year Deliverables: Preliminary studies will be completed providing a basis and proof of concept for the evolution of emergent hierarchical structure for the following work.

End of Project Deliverables: Development of an understanding of the process parameters involved in controlling multi-hierarchical structures in filled elastomers particularly the control of this complex structure with aging time. Correlation between frequency dependent and DC conductivity and the dual hierarchical network.

2) Control of hierarchical structure in skin.

Proposed Team: Y. Park, R. Larson, J. Nickels, A. Jayaraman, D. Pochan; Procter & Gamble, Johnson & Johnson.

Project Objectives: Stratum corneum (SC), a sophisticated outermost skin layer, consists of corneocytes and lipid bilayers in a 'brick and mortar' hierarchical structure. [19] Corneocytes are composed of keratin filaments, natural moisturizing factors, and water. Corneocytes are riveted together by intercellular protein structures called corneodesmosomes, which are keratin filament networks that contain cell adhesion molecules. After washing with cleansers which contain surfactants, our skin 'feels' hydration (or dehydration), or smoothness (or tightness). [20] We ***hypothesize*** that surfactant adsorbs on SC, especially keratin filaments, during washing, and it increases lubrication on the skin surface while surfactant accelerates water loss from the skin because it adsorbs on keratin and lipid and alters the structure. In other words, surfactant adsorbed on keratin may accelerate dehydration but increase lubrication. Our specific objectives are: 1. Develop stratum corneum substitute (SCS) by using synthetic lipids with keratin protein. 2. Determine interplay between molecular level dynamics and macroscale property changes via various analytical tools, including FT-IR, Neutron scattering, X-ray scattering, quasielastic neutron scattering, NMR, dynamic viscoelastic properties of model skin. 3. Develop theoretical models and simulation capabilities to understand the role of surfactants on skin.

Industrial Relevance: The impact of skin care formulas on the hierarchical structures in skin is of pivotal commercial relevance to P&G and several other companies.

Center Relevance: The Center is interested in biological hierarchies and biomimicry.

Experimental Plan: The first part of the study will focus on validating our synthetic SCS model as a testing platform and identifying the effect of various surfactants on structural changes. Our preliminary data with Proctor & Gamble (P&G) demonstrates that our SCS, containing three kinds of lipids and keratin, showed the same characteristics as an actual human stratum corneum in wide angle and small angle x-ray scattering, indicating the lateral and lamellar packing is similar. Our preliminary data in dehydration rate study revealed that keratin plays an important role on dehydration rate, probably due to water binding sites in keratin coil structures which can be measured with dynamic neutron scattering. Cryo-TEM will be pivotal to understanding the scattering and dynamic viscoelastic data.

Milestones and Time to Completion: The project will involve biweekly meetings of the project participants to discuss progress. Organization of neutron scattering beam time and travel to neutron scattering measurements will require approximately 8 months lead time with approximately 3 months for data reduction and analysis. It is anticipated that the project will run a total of 3 years with the last year focusing on publication of results and completion of experiments.

Annual and Total Cost to Completion: The project will require two graduate students at the University of Cincinnati and one at the University of Michigan. The approximate cost per year will be $195,000 per year, total cost of $585,000.

First Year Deliverables: Set up of model skin, preliminary measurements in the three labs.

End of Project Deliverables: Overall, the study will reveal mechanisms behind macroproperties or 'feel' in cosmetics or skin science. At the successful completion of the study we expect the results will significantly impact cosmetics and society as a whole because no study has focused on the molecular mechanisms for skin behavior. Collaboration between research groups at the University of Cincinnati and Michigan and P&G and Johnson & Johnson will generate a synergetic outcome.

3) Biobased hierarchical nanomaterials and nanocomposites

Proposed Team: D. Pochan, A. Jayaraman, Y. Park; Merck, Dupont, Ethicon Endosurgery.

Project Objectives: The development of hybrid nanomaterials/nanoparticles is crucial for the successful encapsulation of desired therapeutic and imaging payloads, desired delivery and stability of the particle and payload, and desired responsiveness of the particle to desired stimuli (e.g. pH, light, ligand binding). The complexity of structure and function observed among protein-based biological, solution-assembled structures lies in stark contrast to the relative simplicity of most synthetic polymer or small molecule amphiphile assembled systems (e.g. nanoscale spheres, cylinders, disks, and vesicles), particularly when simple assembly conditions are employed (neat or low-salt aqueous environments, organic solvents). For example, viruses result from the assembly of a few proteins into specific, yet complicated, nanostructures, whose natural functions include encapsulation and protection, immunological evasion, target binding, and oligonucleotide delivery. With biological molecules, assembly occurs in complex environments that are rich in multiple molecules and undergo temporal changes in composition and structure. This sophistication of protein structures is possible because of 1) information-rich primary structures (i.e. amino acid sequence), 2) defined secondary structures (i.e. molecular conformations such as β-sheets, α-helices, turns and coils) that provide for specific, local shapes and display of amino-acid functionality, 3) specific tertiary, or intramolecular, structures, and 4) well-ordered quaternary, or intermolecular, structures achieved through the assembly of multiple polypeptide chains. We hypothesize that through design of peptides and polypeptides, utilizing natural and non-natural amino acids, we can solution assemble hybrid nanomaterials combining desired structure and function for payload capture, targeting, and function. By combining theory, simulation, and experiment from the University of Delaware and Cincinnati, as well as the hierarchical assembly pathways available in the labs of Pochan and Park, we will be able to develop new nanomaterial vectors based on peptides and polypeptides with other desired materials.

Our specific objectives are: 1. Develop 2-d and 3-d nanomaterials with designed peptides and polypeptides. 2. Determine the hierarchical assembly pathways to combine assembling molecules with desired payload molecules/inorganic nanoparticles/other desired functionality for particle inclusion and form stable, designed nanomaterials. Use analytical tools, including FT-IR, Neutron and X-ray scattering, quasielastic neutron scattering, NMR as well as imaging techniques such as TEM, cryoTEM, and AFM to determine if nanostructure matches those targeted through molecule design and theoretical prediction. 3. Develop further heuristic and theoretical models to predict the molecules needed and hierarchical assembly pathway needed for material formation.

Industrial Relevance: There is a strong need at Merck and Dupont for bionanostructures for new drug and imaging vector development as well as new nanostructures for composite formation to produce other hybrid materials, respectively.

Center Relevance: The Center is interested in biological hierarchies and biomimicry.

Experimental Plan: Initially, desired nanomaterial structure and function will be determined as to target desired properties of the industrial partners. With target structures and functions, peptide or protein molecules can be designed and hierarchical assembly pathways determined for combination with desired payloads and/or co-assembling molecules/particles. Finally, the assembled materials can be studied for desired function in situ/in vitro with potential in vivo study when appropriate.

Milestones and Time to Completion: The project will involve quarterly meetings of the project participants to discuss progress. Organization of neutron scattering and x-ray scattering beam time and travel to neutron scattering measurements will require approximately 8 months lead time with approximately 3 months for data reduction and analysis. It is anticipated that the project will run a total of 3 years with the last year focusing on publication of results and completion of experiments.

Annual and Total Cost to Completion: The project will require two graduate students at the University of Delaware and one at the University of Cincinnati. The approximate cost per year will be $195,000 per year, total cost of $585,000.

First Year Deliverables: Determine initial nanomaterial targets and required molecules for formation. Begin molecule synthesis and initial hierarchical assembly pathway studies.

End of Project Deliverables: The project has the potential to determine significantly different vectors for delivery and/or imaging at Merck using quite different ingredients and processes from traditional delivery vector development. Additionally, new biomolecular nanomaterials will be developed for use in hybrid nanocomposite materials at Dupont and Ethicon.

4) Simulation of emergent macroscopic structure based on experimental nanoscale potentials.

Proposed Team: A. Jayaraman, G. Beaucage; Sun Chemical, Shepherd Color.

Project Objectives: Inks and paints are often composed of surfactant stabilized pigment dispersions [3]. The pigment particles are composed of primary particles that are often on the nanoscale, a size too small to effectively scatter light, that are clustered into aggregates of about 10 to 100 nm size. The size and density of these aggregates depends partly on the primary particle size and the surface interaction between particles in the carrier medium moderated by the surfactant [9]. For organic pigments the primary particles are solid clusters of elemental single crystals whose size depends on the quality of the surfactant/solvent/pigment interface. The system collapses and precipitates at the phase separation temperature of the surfactant. On drying, a controlled collapse of the structure occurs as the concentration increases. For rapid drying in thick films very large 3d particles have been observed to form, which are disadvantageous in application. For drying in micron to hundreds of micron thick films a dual hierarchical network forms composed of clusters of aggregates that from a micron size network in the size range optimal for light scattering. We would like to further demonstrate that this model could apply to a wide range of pigment dispersions and understand control of this emergent structure. This will be achieved by experimentally determining the interaction potential function for pigment elemental, primary, aggregate and agglomerate levels [2, 9]. These potential functions will be used in conjunction with PRISM theory to construct a hierarchical simulation of the formation of this complex structure. The end result will be a predictive software tool where the major variables: surfactant type, drying rate, drying temperature, can be varied and the resulting dual hierarchical structure can be generated. The viability of the tool can be experimentally explored with cryo-TEM and X-ray scattering.

Industrial Relevance: We quote Jeff Peake from Shepherd Color "*As you know, Shepherd Color is a manufacturer of colored inorganic pigments and so understanding the nuances of the structure of our products (not only crystalline structure, but crystallite structure, particle size distribution, agglomerate structure, and dispersion and structure in use) is valuable to us.*" This project addresses these concerns.

Center Relevance: This project ties two groups interested in controlling and understanding the physics and chemistry involved in hierarchical structural emergence in complex systems of commercial importance. The topic and symbiotic approach are in keeping with the intent of CHEM.

Experimental Plan: The experimental materials will be closely tied or aligned with the industrial funders. A baseline for the particular materials will be established by in situ thermal studies using USAXS following references [2, 9]. This will generate potential functions for the different hierarchical levels in the pigment dispersion. These potentials will be used by the Jayaraman group to construct a code that can simulate primary particle growth from crystallites, aggregation, clustering of aggregates and network formation of clusters in a simultaneous fashion. Finally, we will use the simulated structure to compare with scattering structures generated by the methods shown in [7]. The final hierarchical structure will be correlated with optical properties: gloss, haze, translucency, reflectance, brilliance.

Milestones and Time to Completion: The project will involve biweekly meetings of the project participants to discuss progress. Organization of X-ray beam time and travel to X-ray scattering measurements will require approximately 2 months lead time with approximately 3 months for data reduction and analysis. It is anticipated that the project will run a total of 3 years.

Annual and Total Cost to Completion: The project will require a graduate student at the University of Delaware and a graduate student at the University of Cincinnati working in collaboration. The approximate cost per year will be $65,000 per student so a total of $130,000 per year involving two center memberships, total cost of $390,000.

First Year Deliverables: Preliminary studies will be completed providing a basis and proof of concept for the following work.

End of Project Deliverables: Development of an understanding of the process parameters involved in controlling multi-hierarchical structures in pigments particularly the control of this complex structure with processing and application conditions. Correlations will be made between the emergent dual hierarchical structure and ink/paint properties in application.

5) Aramid Ion Transport Membranes.

Proposed Team: N. Kotov, D. Martin; Air Force Research Laboratory

Project Objectives: High-capacity, high-discharge rate batteries are essential for many technologies but their use has been hampered by troublesome safety and longevity records. These problems stem from the growth of dendrites that pierce ion conducting membranes (ITMs) and cause short-circuits leading to capacity fade, overheating, and fires. Attempts at inhibiting dendritic growth for lithium, sodium, zinc, aluminum, and other anodes have met with limited success and highlighted the fact that materials properties needed for safe high-performance batteries are fundamentally difficult to combine.

This project will be focused on unified materials engineering approaches to resolve these problems. It will employ a new method for constructing emergent hierarchical ion-conductors and a new nanoscale component, aramid nanofibers (ANFs). Aramid nanofibers (ANFs) were recently discovered at the University of Michigan as ultra-strong components. We shall evaluate the properties of new ITMs and systematically investigate dendrite suppression for different anode materials and different electrolytes. Dave Martin's group will provide in situ characterization of the aramid fibers. Rapid dissemination of new knowledge about mechanisms of dendrite growth at the ITM-electrode interface will open the door for the development of an ion conductor that can meet the required combination of properties for high-performance batteries.

Industrial Relevance: Lithium ion batteries are of importance to the Air Force mission.

Center Relevance: The Project involves the design and control of an emergent hierarchical structure to improve battery longevity.

Annual and Total Cost to Completion: The project will require two graduate students at the University of Delaware and a graduate student at the University of Michigan working in collaboration. The approximate cost per year will be $65,000 per student so a total of $130,000 per year involving two center memberships, total cost of $390,000.

First Year Deliverables: Preliminary studies will be completed providing a basis and proof of concept for the following work.

End of Project Deliverables: Development of an understanding of the process parameters involved in controlling emergent hierarchical structures in aramid nano-fibers particularly the control of this complex structure with processing and application conditions and battery performance.

6) Hierarchical dynamics of worm-like micelles and coacervates.

Proposed Team: R. Larson, G. Beaucage, N. Wagner; P&G, Dow Agrosciences

Project Objectives: New multi-scale simulation methods and increased computer speed now allow access to time and length scales relevant for commercially important materials. We have made progress towards such simulations of surfactant-containing shampoos, conditioners, and body washes, as well as latex paints which include polymers and colloids, and finally, crystallizing polymers. For polyethylene, we use molecular dynamics simulations and theory to describe the effect of short-chain branches and flow on the rate of nucleation of polyethylene crystals and the effect of long-chain branches on rheology. For worm-like micellar solutions, we use both multi-scale molecular simulations, and micelle-level simulations to determine the effect of micelle properties, including length, stiffness, and entanglement density, on rheological properties. Methods of accelerated sampling, including Umbrella Sampling and Forward Flux Sampling, allow information relevant to long time scales to be extracted from molecular simulations. In all cases, emphasis is on knowledge that could lead to commercial impact. An example of a simulation of breakage of a thread-like micelle, to obtain breakage free energy, and of extraction of micelle parameters from fits to rheological data, are shown in the figure 2. We plan to include structural studies using rheo-SANS at NIST and SANS at ORNL as well as x-ray scattering studies for micelle cross sectional structure to support the parameters using in the simulations.

Industrial Relevance: The study of hierarchical dynamics in WLMs is of primary importance to a wide range of product lines.

Center Relevance: Hierarchical dynamics is an important topic for the center.

Experimental Plan: Samples will be prepared using surfactants chosen by the industrial sponsors such as Sodium laureth sulfate (SLES) and Cocamidopropyl betaine (CAPB). Structural analysis using neutron and X-ray scattering will be conducted in parallel to the simulation and rheology measurements.

Milestones and Time to Completion: The project will involve biweekly meetings of the project participants to discuss progress using computer conferencing. X-ray scattering and parallel rheological experiments will follow approximately the same schedule. The project will run a total of 3 years.

Annual and Total Cost to Completion: The project will require a graduate student at the University of Michigan and a graduate student at the University of Cincinnati working in collaboration. The approximate cost per year will be $65,000 per student so a total of $130,000 per year involving two center memberships, total cost of $390,000.

First Year Deliverables: Preliminary studies will be completed providing a basis and proof of concept for the evolution of emergent hierarchical structure for the following work.

End of Project Deliverables: Development of an understanding of the dynamic hierarchical emergence in WLMs will enable prediction of rheological properties. A software tool will be developed.

Short Courses, Conferences, Targeted Strategy Groups:

The Center for Macromolecular Topology will serve as a forum for the development of ideas and technologies in synthesis, characterization and modeling/simulation of emergent hierarchical structures and dynamics. The center will host a series of short courses aimed at training scientists and engineers in the use of tools developed in the center. Some initial examples of these center sponsored short courses are : "*Simulating hierarchical rheology*" taught by Ron Larson; "*Scattering Techniques for Hierarchical Systems*" taught by Greg Beaucage and Norm Wagner; "*Simulation Methods for Prediction of Thermodynamics and Structure in Hierarchical Systems*" taught by Arthi Jayaraman; "*Synthetic Mechanisms for Surface Modification of Nanoparticles*" Neil Ayres, Jinsang Kim and Anish Tuteja; "*Imaging Techniques for Hierarchical Systems*" Darrin Pochan and Dave Martin.

The Center will also sponsor forums on various aspects of emergent hierarchical systems of interest to the industrial and national lab members. For example a forum on structure/property relationships of skin would be appropriate with invited speakers from outside and inside of the Center. Targeted strategy groups will be developed such as paints and inks group focusing on the characterization and control of nanostructure to build macrostructure on drying. These forum meetings, courses and strategy group meetings would take place just before or just after the Center meetings at the same venue.

Service Contracts:

Some of the facilities and expertise at the Center will be of use in proprietary research by the participating partners and the Center will facilitate service contracts by participating Center members. Some examples of Center based service contracts might involve:

1. **Rheological measurement**. We will use rheological instrumentation available at the University of Michigan, Delaware, and Cincinnati to provide rheological characterization of complex fluids.
2. **Rheological interpretation**. Using advanced modeling methods that account for hierarchical structure, we will interpret the measured rheology.
3. **Rheological training**. Because of short deadlines, and market pressures, industrial practitioners often lack the background needed to use and interpret the latest experimental and theoretical methods in polymer characterization. Training sessions will be offered to regularly bring industrial scientists up to date with the latest methods, drawn from our own work, and that of others from around the world. Unlike rheological short courses offered at other universities, the training we will provide will be tailored to the particular needs of the participating companies, and will address issues raised by them.
4. **Rheological software**. Software, developed at the University of Michigan for interpreting rheological data, will be available including the hierarchical model, as well as improved versions. Efforts will be made to develop software tools that respond to the expressed needs and interests of the industrial participants. Research will be directed towards developing the most useful extensions of existing software, including extensions to polymer solutions, or to polymer containing fillers or additives.
5. **Simulation Tools for Emergent Hierarchical Systems.** The Center will provide a short course in the use of off the shelf software to model complex emergent systems.

Broader Impact:

The Center will actively recruit women, handicapped, and minority graduate and undergraduate students. A REU program focusing on minorities, the handicapped, and women will be associated with the Center with students crossing the three campuses for research work. The center offers the unique education experience of working in a multi-campus team partnering with many industrial partners and national laboratories. Improvement in our control of emergent hierarchical structures will lead directly to improvements in a wide range of consumer and industrial products from hair gels to conveyor belts; from sutures to viscosity enhancers.

Prior NSF:

Prof. David C. Martin: NSF DMR-1808048, "In-situ Transmission Electron Microscopy of the

Electrochemical Deposition of Functionalized Polythiophene Copolymers", 6/2018-6/2021, $441,000.

Intellectual Merit: This research project focuses on development of methods for imaging the transition from liquid monomer to solid polythiophenes due to electrochemical deposition inside a transmission electron microscope with a liquid cell. Establishing this experimental capability has enabled low dose, high resolution TEM studies of the size, shape, and distribution of conjugated polymers during oxidative deposition onto the surface of a thin, conductive, microfabricated electrode. We are now investigating the influence of comonomer chemistry and the addition of solid nanoparticles. These experiments are providing unprecedented new insights about this important process, including the changes in properties and structure that occur as the molecular weight increases. Correlative experiments by complimentary methods including optical microscopy, vibrational spectroscopy, and molecular simulations are making it possible for us to understand the molecular mechanisms of this process in extraordinary detail. *Broader Impact:* The experimental techniques developed in this work would be applicable for investigating hierarchical structural development in a variety of other commercially important, polymer-based products including paints, adhesives, cosmetics, and foodstuffs. The methods would be particularly useful when combined with X-ray or neutron scattering experiments.

Prof. Beaucage: CMMI-1635865 "Collaborative Research: Enabling Design of Polymer Nanocomposites Guided by Mesoscale Simulations and Scattering" $263,991 09/01/2016 to 08/31/19

Intellectual Merit: The objective of the work is to describe nano-dispersion in immiscible systems and use this description to obtain potential functions for use in computer simulations to predict structural outcomes of mechanical mixing. The approach is based on an analogy between thermal dispersion and mechanical dispersion. It was found that while thermal dispersion favors mixing of small nanoparticles; mechanical dispersion favors mixing of large nanoparticles since there is a larger lever arm for dispersion. In the analogy between thermal and mechanical mixing, accumulated strain or mixing time are analogous to temperature. It was possible to write predictive functions for dispersion based on an analogy to the van der Waals equation for the second virial coefficient which yields the excluded volume and the interaction potential between dispersed particles in an elastomer compound under a set mixing geometry. The excluded volume matched the calculated occupied volume plus the bound rubber. The interaction energy, in the context of mechanical mixing, reflects the wetting time required before mixing initiates. We were also able to obtain interaction potentials for mixing. We are in the process of incorporating these potentials into coarse-grain, DPD simulations of nanoparticle dispersion and emergence of hierarchical structure. In this work it was observed that a dual hierarchical structure exists in reinforced elastomers and that this dual hierarchical structure can be directly tied to the dynamic spectrum with characteristic times scaling with characteristic structures in the dual networks. It is believed that this is the first attempt at directly correlating the frequency spectrum with the size spectrum measured in scattering [1]. *Broader Impact:* The project has supported two PhD students (one US Citizen now working at Omya), three undergraduates (one female and one handicapped) and the PI. The project has resulted in nine papers [1-3,7, 9-10, 13-15]. The work was presented at the American Physical Society Meeting in March 2019, 2018, 2017 as well as at the SAS2018 conference in a number of talks and poster presentations. A poster at the SAS2018 meeting won the best poster award.

Prof. Kotov: DMR-1411014 "Ceramic Quasicrystals" $171,122 08/15/14 to 07/31/17

Intellectual Merit: In the last five years, Prof. Kotov led, or participated in, seven NSF grants. The findings of the Kotov research group as a result of NSF funding between 2012-2017 are described in 84 papers published in *Science, Nature Materials, ACS Nano, Angew. Chem., Adv. Mater.,* and others. A total of ten patent applications, including joint patents with industrial collaborators, were filed. The central topic for all his works and outreach activities is biomimetic nanoscale materials and structures with particular emphasis on mechanical properties of nanocomposites. Layer-by-layer assembly technique (LBL) is being used to impregnate ceramic framework to obtain a composite material leading to materials with unusual mechanics and unique toughness. *Broader Impact:* The outreach effort over the course of the #1411014 project consisted of mentoring five female graduate and undergraduate students and post-docs, including three Latino and African Americans.

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Gregory Beaucage, Professor
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati, OH 45221-0012

Office: 513 556-3063
Lab: 513 556-5152
Fax: 513 556-3473
e-mail: beaucag@uc.edu

(a) Professional Preparation

1980 University of Rhode Island, Kingston, RI 02881 ***B.S. Zoology***; Highest Distinction. (Phi Beta Kappa)

1982 University of Rhode Island, Kingston, RI 02881 ***B.S. Chemical Engineering;*** High Distinction. (Phi Kappa Phi)

1991 University of Massachusetts, Amherst, MA 01003 ***Ph.D. Polymer Science and Engineering***. Advisor: ***Richard S. Stein***. *A Morphological, Mechanical and Thermodynamic Investigation of the Isotactic-PVME/PS Polymer Blend.*

1991 Sandia National Laboratory, Albuquerque, NM 87185; ***Post Doctoral Fellow***. Advisors: ***Dale W. Schaefer and John Curro***. Organic Materials Group *Characterization of nanomaterials using scattering & scattering theory.*

(b) Appointments

Paid Appointments:

University of Sheffield, Sheffield UK ***Visiting Professor, Chemical Engineering*** 2018

Fulbright Global Scholar, Sheffield UK, Zürich CH, Cape Town SA, Dire Dawa Ethiopia, Roma Lesotho Funded by the US Department of State. 2017-2019

NanoPower Africa, Cincinnati, OH ***Director*** 2010-2014 http://www.eng.uc.edu/~gbeaucag/NanoPowerAfrica.html

University of Cape Town, South Africa ***Visiting Professor, Physics*** Funded by NanoPower Africa. 1/2010-8/2010.

University of Cincinnati, Cincinnati, OH, 45221 ***Professor***, Department of Chemical and Materials Engineering, 2008-present.

University of Cincinnati, Cincinnati, OH, 45221 ***Associate Professor***, 2000-2007.

ETHZ, Zurich Switzerland ***Visiting Professor, Process Engineering*** Funded by Swiss NSF and Dupont Corporation. 8/2003-8/2004.

University of Cincinnati, Cincinnati, OH, 45221 ***Assistant Professor***, 1994-2000.

Sandia National Laboratory, Albuquerque, NM 87185, ***Staff Member***, Organic Materials Group 1815. Cooperative research agreements with U.S. industrial partners. 1993-1994.

US Patent and Trademark Office, Arlington, VA. ***Patent Examiner*** Biomedical Materials. 1982-1986.

Voluntary Appointments:

SHUG SNS-HFIR User Group Oak Ridge National Laboratory, ***Chair*** 2010-2013, ***Member*** 2008-2015

American Physical Society, Fellow 2008-Present.

Small Angle Scattering Special Interest Group ACryS, ***Chair***, 2004-2005 **Program Chair**, 2003-2004.

LENS Neutron Scattering Facility at Indiana University, ***Founding Member*** 2003-Present.

CAMD SAXS User Group ***Founding Member*** at LSU Synchrotron 2000-Present.

Intense Pulse Neutron Source, Argonne National Laboratory, ***Member Advisory Board***, 2000-2008.

NSF/PRF/DOE/Commerce/State Department, ***Panel and Individual Referee***, 1995-Present.

(**c) Products**

10 Related Publications (from 151 peer reviewed H-Index 34)

1) *Impact of an emergent hierarchical filler network on nanocomposite dynamics* Rishi K, Beaucage G, Kuppa V, et al. *Macromolecules* **51**(20) (2018) 7893-7904. doi: 10.1021/acs.macromol.8b01510.
2) *Structural emergence in particle dispersions.* Mulderig A et al. *Langmuir* **33**(49) (2017) 14029-14037. doi: 10.1021/acs.langmuir.7b03033.
3) *A pseudo-thermodynamic description of dispersion for nanocomposites* Jin Y, Beaucage G, Vogtt K, et al. *Polymer* **129** 32-43 (2017) doi: 10.1016/j.polymer.2017.09.040.
4) *Determination of branch fraction and minimum dimension of mass-fractal aggregates.* Beaucage G, *Phys. Rev. E*, **70**, 031401 (2004). doi: 10.1103/PhysRevE.70.031401
5) *Probing the dynamics of nanoparticle growth in a flame using synchrotron radiation.* Beaucage G, Kammler HK, Agashe N, Pratsinis SE and Narayanan T, *Nature Mater.* **3,** 370-373 (2004). doi: 10.1038/nmat1135
6) *A structural model for equilibrium swollen networks*. Sukumaran SK, Beaucage G *Europhysics Letters* **59** 714-720 (2002). doi: 10.1209/epl/i2002-00184-7
7) *Monitoring simultaneously the growth of nanoparticles and aggregates by in situ ultra-small-angle x-ray scattering.* Kammler HK, Beaucage G, Kohls DJ, Agashe N. Ilavsky J., *J Appl. Phys.* **97**(5) (2005) (Article 054309). doi: 10.1063/1.1855391
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9) *Approxis leading to a unified exponential/power-law approach to small-angle scattering.* Beaucage G, *J. Appl. Cryst.* **28**, 717-728 (1995). doi: 10.1107/S0021889895005292.
10) *Towards resolution of ambiguity for the unfolded state.* Beaucage G *Biophysical J.* **95** 503-509 (2008). doi: 10.1529/biophysj.107.121855.

(d) Synergistic Activities

1) Creation: Fullbright Fellowship 2017-2019 developed technical startup businesses in Ethiopia and Lesotho in collaboration with Addis Ababa University, Dire Dawa University, National University of Lesotho, Cape Town University, University of the Witwatersrand, and the University of Sheffield. Businesses started manufacture soil moisture sensors for drip irrigation, solar street lights, absorption refrigerators, solar production of charcoal from bamboo, and printed electronic solar cells for cell phone charging.

2) Creation: Developed *NanoPower Africa* project coupling five African Universities, two US National Labs, the University of Cincinnati, and NGO and industrial participants in an effort to improve higher education in sub-Saharan Africa and to develop indigenously manufactured photovoltaics.

3) Creation: Development of scattering theories (the unified function) to describe aggregate nanostructures, biopolymers, branched structures [1-4,6-10]. *Integration:* Pioneered application of x-ray scattering in situ to pyrolytic synthesis of nanomaterials [2,3]. *Transfer of Knowledge*: Developed and co-developed user software for the analysis of scattering data using the unified function with Jan Ilavsky at Argonne National Laboratory.

4) Transfer of Knowledge: Chairman of small-angle scattering group American Crystallographic Association, Organizer for annual meeting of ACA. 30 Sessions Organized for AIChE, ACA, MRS, APS, SAS meetings.

5) *Transfer of Knowledge*: 20 web courses extensive notes, lab experiments and data. 900,000 different IP#'s have hit this course suite since 2000 (averaging >100 IP hits/day).

NEIL AYRES, PH. D.

A. PROFESSIONAL PREPARATION

University of Warwick, Coventry, U.K.	Chemistry	B.Sc. 1999
University of Warwick, Coventry, U.K.	Chemistry	Ph.D. 2003
University of Southern Mississippi, Hattiesburg, MS	Polymer Science	(Post Doc) 2003-2004
University of Akron, Akron, OH	Polymer Science	(Post Doc) 2004-2006
University of Utah, Salt Lake City, UT	Bioengineering	(Post Doc) 2006-2008

B. APPOINTMENTS

2014-present Associate Professor, University of Cincinnati, Department of Chemistry.
2008-2014 Assistant Professor, University of Cincinnati, Department of Chemistry.

C. PRODUCTS

(i) Products closely related to this proposal

1. M. Mario Perera and Neil Ayres (2017) *Gelatin based dynamic hydrogels via thiol-norbornene reactions* Polymer Chemistry, 8, 6741-6749
2. Niranga Wijesiri, Tevhide Ozkaya-Ahmadov, Peng Wang, Jinnan Zhang, Hong Tang, Xinjun Yu, Neil Ayres, and Peng Zhang (2017) *Photodynamic inactivation of multidrug-resistant Staphylococcus aureus using hybrid photosensitizers based on amphiphilic block copolymer-functionalized gold nanoparticles* ACS Omega, 2, 5364-5369
3. Xinjun Yu, Xiaoping Chen, Qinyuan Chai and Neil Ayres (2016) *Synthesis of polymer organogelators using hydrogen bonding as physical cross-links* Colloid and Polymer Science 294 (1) 59-68
4. Xiaoping Chen, Pengzhan Fei, Kevin A Cavicchi, Wenwen Yang, and Neil Ayres (2014) *The poor solubility of ureidopyrimidone can be used to form gels of low molecular weight N-alkyl urea oligomers in organic solvents* Colloid and Polymer Science, 292, 477-484
5. Leeanne Taylor, Xiaoping Chen, and Neil Ayres (2014) *Synthesis of a glycosaminoglycan polymer mimetic using an N-alkyl-N,N-linked urea oligomer containing glucose pendant groups* Polymer International 63 127-135

(ii) Other significant products

1. Qinyuan Chai, Yongshun Huang, Terrence Kirley, and Neil Ayres (2017) *Shape memory polymer foams prepared from a heparin-inspired polyurethane/urea*, Polymer Chemistry, 8, 5039-5048
2. Yongshun Huang, Maureen A. Shaw, Mary R. Warmin, Eric S. Mullins, and Neil Ayres (2016) *Blood Compatibility of heparin-inspired, lactose containing, polyureas depends on the chemistry of the polymer backbone* Polymer Chemistry, 7, 3897-3905
3. Yongshun Huang, Maureen A. Shaw, Eric S. Mullins, Terence L. Kirley, and Neil Ayres (2014) *Synthesis and Anticoagulant Activity of Polyureas Containing Sulfated Carbohydrates* Biomacromolecules, 15, 4455-4466
4. Yongshun Huang, Leeanne Taylor, Xiaoping Chen, and Neil Ayres (2013) *Synthesis of a polyurea from a glucose or mannose containing N-alkyl urea peptoid oligomer* Journal of Polymer Science, Part A: Polymer Chemistry 51(24) 5230-5238

5. Xiaoping Chen and Neil Ayres (2010) *Synthesis of Novel Polymer/Urea Peptoid Conjugates using RAFT polymerization* Macromolecules, 43, 1341-1348

D. SYNERGISTIC ACTIVITIES

1. Dr. Ayres has a secondary faculty appointment in the **Materials Science and Engineering program** within the College of Engineering and Applied Science at the University of Cincinnati.
2. Dr. Ayres is the "**Bordeaux Connections Director**" in the Department of Chemistry at UC, and has led two faculty-lead study abroad trips to the University of Bordeaux, FR.
3. Dr. Ayres attended University of Cincinnati's *Center for Enhancement of Teaching & Learning* workshops on course redesign for active learning, just-in-time teaching practices, Getting Started with Echo360 ALP, The Science of Motivation: Pedagogy and Student Engagement, and teaching large lecture courses.
4. Dr. Ayres has mentored six undergraduate students as part of the UC's Department of Chemistry's **NSF REU** program
5. Dr. Ayres was a member of the University of Cincinnati's McMicken College of Arts and Science's *Instructional Innovations Advisory Council* in 2015-2016.

Jonathan D. Nickels
Assistant Professor
Department of Chemical and Environmental Engineering
The University of Cincinnati
(513) 556-3938, jonathan.nickels@uc.edu

Professional Preparation

The University of Notre Dame	South Bend, IN	Chemical Engineering	BS, 2004
The University of Texas at Austin	Austin, TX	Biomedical Engineering	PhD, 2009
Oak Ridge National Laboratory	Oak Ridge, TN	Neutron Scattering and Biophysics	Postdoctoral, 2010-2017.

Appointments

Assistant Professor, The University of Cincinnati, Department of Chemical and Environmental Engineering, 2017- current.

Products

Related Products

1. Perticaroli S, Ehlers G, Stanley CB, Mamontov E, O'Neill H, Zhang Q, Cheng X, Myles DA, Katsaras J, **Nickels JD**. Description of Hydration Water in Protein (Green Fluorescent Protein) Solution. *Journal of the American Chemical Society*. 2017;139(3):1098-105. DOI: 10.1021/jacs.6b08845
2. **Nickels JD**, Cheng X, Mostofian B, Stanley C, Lindner B, Heberle FA, Perticaroli S, Feygenson M, Egami T, Standaert RF. Mechanical properties of nanoscopic lipid domains. *Journal of the American Chemical Society*. 2015;137(50):15772-80. DOI: 10.1021/jacs.5b08894
3. Perticaroli S, Mostofian B, Ehlers G, Neuefeind JC, Diallo SO, Stanley CB, Daemen L, Egami T, Katsaras J, Cheng X, **Nickels JD**. Structural relaxation, viscosity, and network connectivity in a hydrogen bonding liquid. *Physical Chemistry Chemical Physics*. 2017; 19 (38), 25859-25869. DOI: 10.1039/C7CP04013J
4. **Nickels JD**, Atkinson J, Papp-Szabo E, Stanley C, Diallo SO, Perticaroli S, Baylis B, Mahon P, Ehlers G, Katsaras J. Structure and hydration of highly-branched, monodisperse phytoglycogen nanoparticles. *Biomacromolecules*. 2016;17(3):735-43. DOI: 10.1021/acs.biomac.5b01393
5. Perticaroli S, Ehlers G, Jalarvo N, Katsaras J, **Nickels JD**. Elasticity and inverse temperature transition in elastin. *The Journal of Physical Chemistry Letters*. 2015;6(20):4018-25. DOI: 10.1021/acs.jpclett.5b01890

Other Significant Products

1. **Nickels JD**, Chatterjee S, Stanley CB, Qian S, Cheng X, Myles DA, Standaert RF, Elkins JG, Katsaras J. The in vivo structure of biological membranes and evidence for lipid domains. *PLoS Biology*. 2017;15(5):e2002214.DOI: 10.1371/journal.pbio.2002214
2. **Nickels JD**, Chatterjee S, Mostofian B, Stanley CB, Ohl M, Zolnierczuk P, Schulz R, Myles DA, Standaert RF, Elkins J. The Bacillus Subtilis Lipid Extract, A Branched-Chain Fatty Acid Model Membrane. *The Journal of Physical Chemistry Letters*. 2017; 8 (17), 4214-4217. DOI: 10.1021/acs.jpclett.7b01877

3. **Nickels JD**, Smith MD, Alsop RJ, Himbert S, Yahya A, Cordner D, Zolnierczuk P, Stanley CB, Katsaras J, Cheng X, Rheinstädter MC. Lipid Rafts: Buffers of Cell Membrane Physical Properties. *Journal of Physical Chemistry B*. 2019; 123(9):2050-2056. DOI: 10.1021/acs.jpcb.8b12126.
4. **Nickels JD**, Perticaroli S, O'Neill H, Zhang Q, Ehlers G, Sokolov AP. Coherent Neutron Scattering and Collective Dynamics in the Protein, GFP. *Biophysical Journal*. 2013; 105 (9), 2182-2187. DOI: 10.1016/j.bpj.2013.09.029
5. **Nickels JD**, O'Neill H, Hong L, Tyagi M, Ehlers G, Weiss KL, Zhang Q, Yi Z, Mamontov E, Smith JC. Dynamics of protein and its hydration water: neutron scattering studies on fully deuterated GFP. *Biophysical Journal*. 2012;103(7):1566-75. DOI: 10.1016/j.bpj.2012.08.046

Synergistic Activities

1. National meeting leadership/organization, served as: Session Co-Chair of Biomembranes Symposium at ACS National Meeting (Spring – 2017-19).
2. National meeting leadership/organization, served as: Session Co-Chair of Biological Structures and Dynamics at ACNS (2018).
3. Visiting Instructor: ORNL Neutrons in Structural Biology Symposium (2016,18)
4. Volunteer activities such as Judge with Buckeye (statewide) Science and Engineering Fair (2018)
5. Review activities such as serving on the On-Site neutron beamtime allocation committee at ORNL Spallation Neutron Source (2017-19), NSF ad-hoc (2018-19).

YOONJEE PARK, PhD

(a) PROFESSIONAL PREPARATION

Seoul National University	Chemical & Biological Engineering	B.S. 2006
Purdue University	Chemical Engineering	Ph.D. 2010
Boston University	Biomedical Engineering	Postdoc, 2010-2013
Massachusetts Institute of Technology	Biological Engineering	Postdoc, 2013-2014

(b) APPOINTMENTS

Assistant Professor	University of Cincinnati	Cincinnati, OH	2015-present
Postdoctoral Associate	MIT	Cambridge, MA	2013-2014
Postdoctoral Associate	Boston University	Boston, MA	2010-2013
Graduate Research Associate	Purdue University	West Lafayette, IN	2006-2010
Undergraduate Research Assistant	Seoul National University	Seoul, Korea	2005-2006

(c) PRODUCTS

i) Five related products to the proposed project

Zhang, Z., Taylor, M., Kaval, N., **Park, Y.** "Phase-transition kinetics of gold nanorod-coated nanodroplets for understanding plasmonic heat by pulsed laser", *The Journal of Physical Chemistry A*, (2019).

Zhang, Z., Taylor M., Collins C., Haworth, S., Shi, Z., Yuan, Z., He, X., Cao, Z., **Park, Y.C.** "Light-Activatable Theranostic Agents for Image-Monitored Controlled Drug Delivery", *ACS Applied Materials and Interfaces,* 10 (2) 1534-1543 (2018).

Nguyen, K., Pan, H.-Y., Mahoney, E., Mercado, K., Haworth, K., Lin, C.-Y., **Park, Y**.**C**. "On-demand Drug Release via High-Intensity Focused Ultrasound for Chronic Disc Degeneration Treatment", accepted, *Ultrasound in Medicine and Biology* (2018).

Park, Y.C., Zhang, C., Kim, S., Mohamedi, G., Beigie, C., Nagy, J. O., Jeon, N.L., Holt, R. G., Wong, J. Y. "Microvessels-on-a-Chip to Assess Targeted Ultrasound-Assisted Drug Delivery," *ACS Applied Materials and Interfaces*, 8, 31541-31549 (2016).

Park, Y., Luce, A. C., Whitaker, R. D., Amin, B., Cabodi, M., Nap, R., Szleifer, I., Cleveland, R. O., Nagy, J. O., Wong, J. Y. "Tunable Diacetylene Polymerized Shell Microbubbles as Ultrasound Contrast Agents," *Langmuir*, vol. 28 (8) 3766-3772 (2012).

ii) Five other significant products

Ventura, S. Heikenfeld, J., Brooks, T., Esfandiari, L., Boyce, S., **Park, Y**., Kasting, G.B. "Cortisol extraction through human skin by reverse iontophoresis," *Bioelectrochemistry,* vol. 114, 54–60 (2017).

Park, Y.C.*, Pham, T.*, Beigie, C., Cabodi, M., Cleveland, R. O., Nagy, J. O., and Wong, J. Y. "Generation of Monodisperse Micro-Oil Droplets Stabilized by Polymerizable Phospholipid Coatings as Potential Drug Carriers," *Langmuir*, 31, 9762−9770 (2015).

Park, Y.C.*, Smith, J. B.*, R.D. Whitaker, T. Pham, C. Sucato, J.A. Hamilton, E. Bartolak-Suki, and J.Y. Wong, "Effect of PEG Molecular Weight on Stability, T_2 contrast, Cytotoxicity, and Cellular Uptake of Superparamagnetic Iron Oxide Nanoparticles (SPIONs)" *Colloids and Surfaces B: Biointerfaces*, 119: 106-114 (2014).

Park, Y., Whitaker, R. D., Nap, R., Paulsen, J., Mathiyazhagan, V., Doerrer, L. H., Song, Y.-Q., Hurlimann, M., Szleifer, I., and Wong, J. Y. "Stability of Superparamagnetic Iron Oxide Nanoparticles at Different pH Values: Experimental and Theoretical Analysis," *Langmuir*, vol. 28 (15) 6246-6255 (2012).

Park, Y., Huang, R., Corti, D.S., and Franses, E.I. "Colloidal Dispersion Stability of Unilamellar DPPC Vesicles in Aqueous Electrolyte Solutions and Comparisons to Predictions from the DLVO Theory," *Journal of Colloid and Interface Science*, vol. 342 (2) 300-310 (2010).

(d) SYNERGISTIC ACTIVITIES

Editorial board and Reviewer: Korean Chemical Engineering Research (2017–present) Langmuir; ACS Applied Materials & Interfaces, Theranostics, Expert Opinion on Drug Delivery; Soft Matter; Scientific Reports; Journal of Controlled Release; Journal of Pharmaceutical and Biomedical Analysis; Biotechnology and Bioprocess Engineering; Advances in Colloid and Interface Science; Journal of Magnetic Resonance Imaging; Applied Biochemistry and Biotechnology; Materials.

Conference/workshop organizing committee: Park served as a session chair at UKC (US-Korea Conference) 2015 in Biomaterials and Nanotechnology session, and UKC 2016 in Nanotechnology session. I invited speakers who are actively doing research in the US and in Korea. Park served as a session co-chairs at 2017-2019 AIChE national meeting in Colloidal Dispersions and Drug/Gene Delivery sessions.

Board member of professional society: Park has served as a Director of Young Generation Affairs in KIChE (Korean Institute of Chemical Engineers) US Chapter since 2011 to enhance academic and professional promotion of the Korean and Korean-American chemical engineers through events at AIChE (American Institute of Chemical Engineers) annual meetings.

Broadening participation of researchers from underrepresented groups: Park has advised and mentored more than ten female undergraduate and graduate students in STEM disciplines. One of them was African American. Park helped female undergraduate students continue their career and enter graduate programs. Also Park partnered with Cincinnati Museum Center to give lectures and hand-on experiment on Nanoscience to K-12 girls.

Awardee: Park recently received awards based on research, education, and service efforts, including "KIChE President Young Investigator Award" in 2015, "Health Research Rising Start Award" at UC in 2016, "Ohio Lions Eye Research Foundation AMD Award" in 2017, "NIH KL2 Scholarship Award" in 2018.

Center for Hierarchical Emergent Materials
Proposed Center Marketing Plan

Target Industries: The target industries for the CHEM are: 1) the organic pigment industry; 2) the inorganic pigment industry; 3) paint industry; 4) ink industry; 5) the elastomer and rubber industries and producers of reinforcing fillers; 3) consumer products industry; 4) biomedical devices and drug delivery industry; 5) adhesives industry; 6) coatings industry; 7) catalyst support industry; 8) plastics compounding industry.

Marketing Plan: The marketing plan will be fully developed at the Planning Meeting. Currently the Center is being marketed through personnel contacts of the co-PI's and through initiation of new contacts via networking.

We plan to develop a web page for the Center that will include interactive components for marketing of the Center. We also plan to present the Center at meetings of the American Institute of Chemical Engineers, Society of Plastics Engineers (ANTEC) and other meetings where it is likely that industrial research and development scientists and engineers working in this area may be likely to attend such as the Color Pigments Manufacturers Association (CPMA). The Center will offer short courses and forums that will draw potential members. The Directors will market the Center to attendees of these meetings and courses.

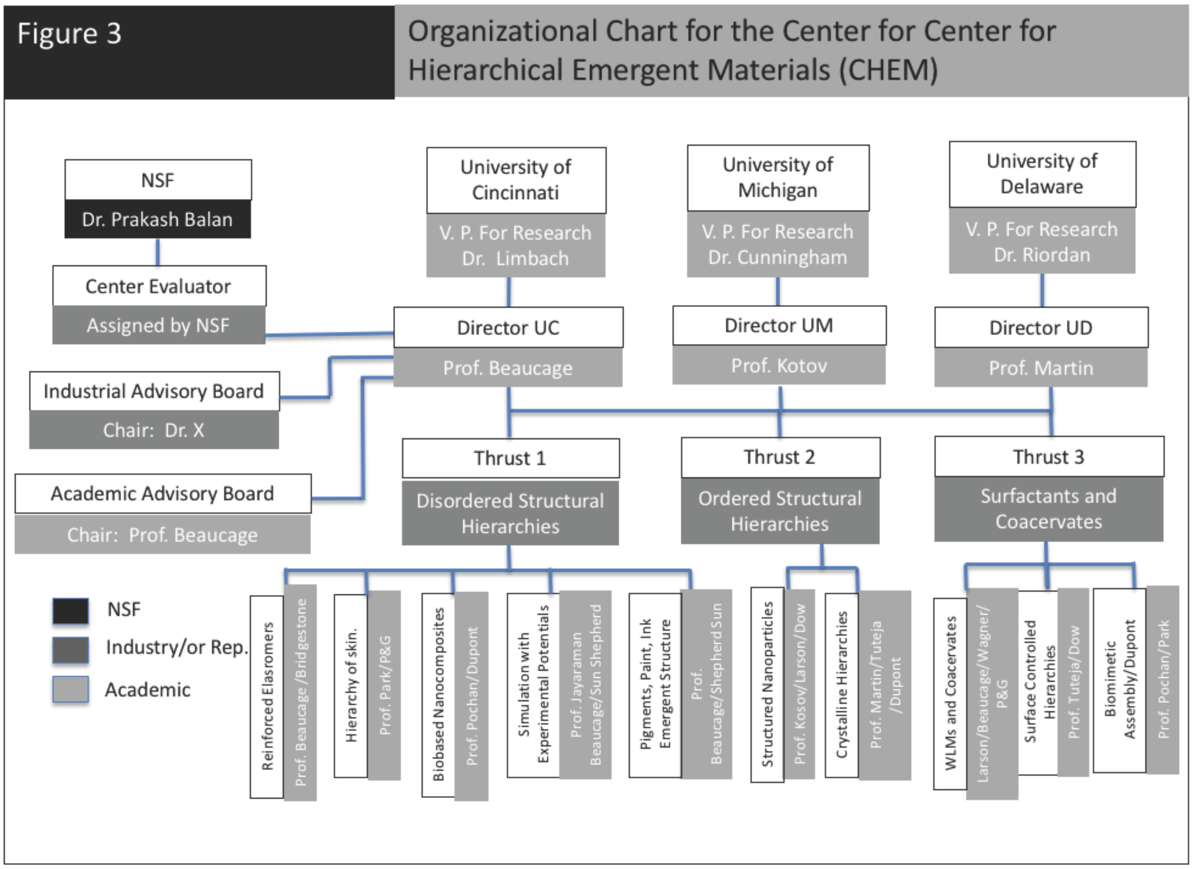
For the most part, marketing of the Center will be the task of the three Center Directors and especially the lead Director at Cincinnati. Researchers interested in participating in the Center at the participating Universities will be encouraged to bring sponsors to the Center and in the absence of sponsors, the Center will attempt to find sponsors who can support the proposed research or suggest projects that can effectively partner university expertise with industrial interests. The Center will initially have several projects supporting the founding academic member's research interests that will form the core of the Center Site sponsorships required by NSF.

Center Growth: It is expected that the Center will add two companies per year as full members in the first five years with an attrition rate of one company per 3 years (at the end of a typical project). If the Center begins with 12 full members, the Center could grow to 15 or 16 members after 5 years supporting about 10 to 12 faculty at the two universities.

Participation in the Center: Center participation mechanisms will be discussed at the planning meeting and will be decided taking into account discussions at that meeting. One successful approach is to copy the membership mechanisms used by the IRC at the University of Leeds in the UK (http://phyast4.leeds.ac.uk/pages/TheIndustrialClub). In this scenario a bare Center membership is offered for about $10,000 that would allow attendance at Center meetings, forums and short courses. To buy into a research project a Full Membership would be required which would cost a minimum of $65,000 to support one student. For National Lab members and members intending to contribute to the research effort of the Center some type of in kind cost sharing may be possible. This would be done on a case-by-case basis at the approval of the industrial and academic boards. The complexities of these membership types will only be worked out with discussion at the planning meeting and finally by a trial and error process. The goal of the Center will be to broaden the membership as far as possible while maintaining a functional center and allowing proportional representation on Center decisions based on the financial contributions to the Center effort.

Staffing Plan for The Center for Hierarchical Emergent Materials

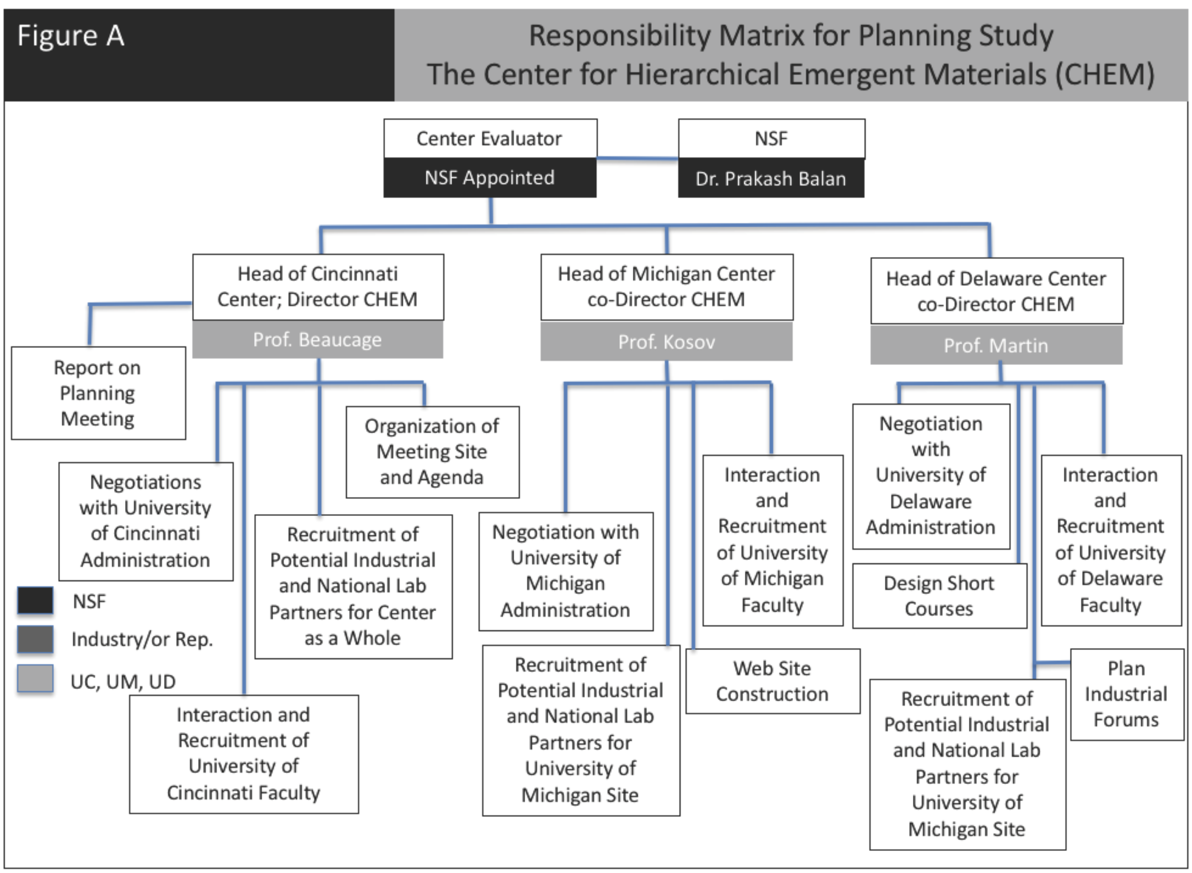
Figure 3, from the Project Description (reproduced below), shows the proposed Organizational Chart for the Center for Hierarchical Emergent Materials (CHEM).



The Center for Hierarchical Emergent Materials will have three sites, at the University of Cincinnati, the University of Delaware and at the University of Michigan. The Center Director and co-Director will report to their respective Vice Presidents for Research concerning issues of importance to the University such as University support for the research efforts associated with the Center. The Center Director at Cincinnati will have the main administrative functions in dealing with the National Science Foundation and the two Advisory Committees: The Industrial Advisory Committee and the Academic Advisory Committee. The Academic Advisory Committee will be chaired by Prof. Beaucage. Dr. Ryan Breese from LyondellBasell will Chair the Industrial Advisory Board. Dr. Breese is a senior researcher at LyondellBasell in Cincinnati and is an officer in the Society of Plastics Engineers. The Center Directors will oversee the three main thrusts of disordered hierarchies, ordered hierarchies and surfactants/coacervates. Activities in all three of these thrusts will exist at the three campuses. Efforts will be made to develop projects that have components on multiple campuses. Each research thrust will have an Oversight Committee composed mostly of industrial/national lab scientists and engineers associated with projects in the Thrust. The Oversight Committees will report to the Directors. Each Thrust

Oversight Committee will support a number of research projects that can have multiple PI's. A Center Evaluator will assess the operation of the Center and report to the NSF Program Manager.

Responsibility Matrix for the planning study: Figure A, below, shows the responsibility matrix for the planning study. Profs. Beaucage, Martin, and Kotov will be primarily responsible for the planning study. Beaucage will organize the planning meeting and agenda as specified in the Project Description. Beaucage will also be responsible for interaction with the administration at the University of Cincinnati and in recruiting faculty members to participate in the center. Beaucage will coordinate recruitment of industrial and national lab partners for the Center. Prof. Kotov will interact with the University of Michigan administration and faculty and will recruit industrial and national lab partners for the Michigan site. Prof. Martin will perform the same duties at Delaware. Martin will also take primary responsibility for oversite of the design of short courses and industrial forums within the center. Prof. Kotov will construct a Center web page. Beaucage will prepare a report on the planning meeting that will be posted on the web page. The Center Evaluator will assess the planning meeting and will prepare a report for the NSF program manager.



Draft Membership Agreement for Industrial Partners
for The Center for Hierarchical Emergent Materials

This Agreement is made..........this day of ...... by and between the University of Cincinnati/Michigan/Delaware (hereinafter called "University") and … (hereinafter called "Company") for the Center comprising and acting through The Center for Hierarchical Emergent Materials (hereinafter called "CENTER"), which is defined as all CENTER Research Sites funded by the Industry/University Cooperative Research Center Program of the National Science Foundation.

WHEREAS, the parties to this Agreement intend to join together in a cooperative effort to support an Industry/University Cooperative Research Center for Hierarchical Emergent Materials at the UNIVERSITY to maintain a mechanism whereby the UNIVERSITY environment can be used to perform research to advance our understanding of complex hierarchical emergent materials. The parties hereby agree to the following terms and conditions:

A. CENTER will be operated by certain faculty, staff and students at the UNIVERSITY. For the first five years, the CENTER will be supported jointly by industrial firms, Federal laboratories, the National Science Foundation (NSF), the States of Ohio and Michigan, and the UNIVERSITY. It is possible that the UNIVERSITY may receive support from NSF for an additional ten years.
B. Any COMPANY, Federal Research and Development organization, or any Government-owned Contractor Operated laboratory may become a sponsor of the CENTER, consistent with applicable state and federal laws and statutes.

C. COMPANY agrees to contribute $65,000 annually in support of the CENTER and thereby becomes a member. Payment of these membership fees shall be made to the University of Cincinnati or Michigan as a lump sum effective___; or in four equal quarterly installments on _____, ____, ____ and ____ of each year of sponsorship. Checks from COMPANY should be mailed to ___ and made payable to _____. Because research of the type to be done by the CENTER takes time and research results may not be obvious immediately, COMPANY should join CENTER with the intention of remaining a fee-paying member with full voting rights for at least two years. However, COMPANY may terminate this Agreement by giving UNIVERSITY 90 days written notice prior to the termination date.
D. There will be an Industrial Advisory Board composed of one representative from each member. This board makes recommendations on (a) the research projects to be carried out by CENTER (b) the apportionment of resources to these research projects, and (c) changes in the bylaws.

E. UNIVERSITY reserves the right to publish in scientific or engineering journals the results of any research performed by CENTER. COMPANY, however, shall have the opportunity to review any paper or presentation containing results of the research program of CENTER prior to publication of the paper, and shall have the right to request a delay in publication for a period not to exceed 1 year from the date of submission to COMPANY, for proprietary reasons, provided that COMPANY makes a written request and justification for such delay within 45 days from the date the proposed publication is submitted by certified mail to COMPANY.

F. All patents derived from inventions conceived or first actually reduced to practice in the course of research conducted by the CENTER shall belong to UNIVERSITY. UNIVERSITY, pursuant to chapter 18 of title 35 of the United States Code, commonly called the Bayh-Dole Act, will have ownership of all patents developed from this work, subject to "march-in" rights as set forth in this Act.

G. UNIVERSITY agrees that all such CENTER sponsors are entitled to a nonexclusive royalty-free license. COMPANY will have the right to sublicense its subsidiaries and affiliates. COMPANIES that wish to exercise rights to a royalty-free license agree to pay for the costs of patent application.

H. If only one COMPANY seeks a license, that COMPANY may obtain an exclusive fee-bearing license through one of its agents. COMPANY has the right to sublicense its subsidiaries and affiliates.

I. Copyright registration shall be obtained for software developed by CENTER. COMPANY shall be entitled to a nonexclusive, royalty-free license to all software developed by CENTER. COMPANY will have the right to enhance and to re-market enhanced or unenhanced software with royalties due to CENTER to be negotiated, based on the worth of the initial software, but not to exceed __% of a fair sale price of the enhanced software product sold or licensed by COMPANY.

J. Any royalties and fees received by UNIVERSITY under this Agreement, over and above expenses incurred, will be distributed as follows: (1) ___% to inventor, or in accordance with UNIVERSITY royalty sharing schedule, (2) ___% to the University of ___, and (3) __ % to the CENTER operating account, or to the College of ___ in the event that CENTER is no longer in operation.

K. Neither party is assuming any liability for the actions or omissions of the other party. Each party will indemnify and hold the other party harmless against all claims, liability, injury, damage or cost based upon injury or death to persons, or loss of, damage to, or loss of use of property that arises out of the performance of this agreement to the extent that such claims, liability, damage, cost or expense results from the negligence of a party's agents or employees.

Draft Membership Agreement for Associations and Institutions
Center for Hierarchical Emergent Materials (CHEM)

This Agreement ("Dissemination Agreement") is made this _______ day of ___________, 2020 by and between the University of Cincinnati/University of Michigan/University of Delaware (hereinafter "University") acting on behalf of The Center for Hierarchical Emergent Materials and the undersigned Center for Hierarchical Emergent Materials_ Member ("Member").

WHEREAS, Center for Hierarchical Emergent Materials conducts research projects which are funded by its Members pursuant to the Industry/University Cooperative Research Center for Center for Hierarchical Emergent Materials ("Membership Agreement") placed into effect between University and each Member; and

WHEREAS, the undersigned Center for Hierarchical Emergent Materials Member entered into the Membership Agreement effective as of ____________________; and

WHEREAS Center for Hierarchical Emergent Materials and its Members desire to disseminate to the public, non-confidential, general information and non-confidential research results generated from the research projects;

NOW, therefore, the parties to this Dissemination Agreement hereby agree to the following terms and conditions governing public dissemination of non-confidential information:

A. Each Member shall receive the following:

i) The right to select one (1) research project of Member's choice.

ii) A written report, for Member's internal-use only for each ongoing Center for Hierarchical Emergent Materials Center project, to be delivered prior to each periodic meeting with Members of Center for Hierarchical Emergent Materials Center, and following each periodic meeting, access to the oral presentation given for each project.

iii) In a timely manner following each periodic meeting, an executive summary report providing information of a general, non-confidential nature about the progress of the research projects, including the right to copy, republish, and distribute, in whole or in part, the report to all interested members of the public.

iv) To the extent permitted by the Membership Agreement's provisions for preserving patent rights, six months after the completion of a Center for Hierarchical Emergent Materials Center project, non-confidential results of the project including the right to copy, republish, and distribute, in whole or in part, the results to all interested members of the public.

B. This Agreement may not be assigned, in whole or in part, by either party without the prior written consent of the other party; and such consent shall not be unreasonably withheld.

C. The terms and conditions of the Membership Agreement are incorporated herein, and the terms and conditions above are supplemental to the terms and conditions of the Membership Agreement. In the event of any conflict between the terms and conditions of this Dissemination Agreement and the terms and conditions in the Membership Agreement, the terms and conditions of the Membership Agreement shall prevail.

IN WITNESS WHEREOF, the parties hereto have caused this Dissemination Agreement to be executed by their duly authorized representatives.

University

Name: ______________________________

Title: ______________________________

Signature: ______________________________

Date: ______________________________

Member: NAME OF ASSOCIATION.

Name: ______________________________

Title: ______________________________

Signature: ______________________________

Date: ______________________________

Center for Hierarchical Emergent Materials
Draft Planning Meeting Agenda
Kingsgate Marriott, University of Cincinnati, Cincinnati, OH

Day 1:

7:30 am	Participant registration
7:30 - 8:15 am	Breakfast and social time
8:15 - 8:35 am	Welcome remarks: Prof. Greg Beaucage, Prof. Dave Martin, Prof. Nick Kotov Pat Limbach, Vice President of Research, University of Cincinnati Patrick Limbaugh, Vice Provost and Dean of the Graduate School, Univ. Cincinnati Representatives from the University of Michigan and Delaware
8:35 - 9:15 am	Vision and Capabilities of the Center (Prof. Greg Beaucage, Prof. Dave Martin, Prof. Nick Kotov)
9:15 - 10:00 am	NSF I/UCRC presentation: I/UCRC Program Director and Evaluator
10:00 - 10:15 am	**BREAK**
10:15 - 12:15 pm	**Project Presentations (Thrust 1: Disordered Hierarchies)** Limit to 5 projects; list the project titles and time allocated to each; make sure that each project has deliverables (especially for the first year), milestones and proposed budget; also, make sure that LIFE forms are filled out at the end of each presentation, and all are collected at the end of each session.
12:15 - 1:00 pm	**LUNCH**
1:00 - 3:00 pm	**Project Presentations (Thrust 2: Ordered Hierarchies; Thrust 3)** Limit to 5 projects; list the project titles and time allocated to each; make sure that each project has deliverables (especially for the first year), milestones and proposed budget; also, make sure that LIFE forms are filled out at the end of each presentation, and all are collected at the end of each session
3:00 - 3:15 pm	**BREAK**
3:15 - 4:30 pm	Industry Workshop (involves discussion of projects & company needs NOT addressed in the above Project Presentations)
4:30 - 4:45 pm	Review of evening and Day 2 activities (Profs. Dave Martin, Greg Beaucage, Nick Kotov)
6:00 pm	Technical Forum and Social: Poster Session Posters of proposed projects, we expect ~10 from each University.

Day 2:

7:30 - 8:00 am
Arrival and Breakfast

8:00 - 9:30 am
Feedback from Industry Workshop - Industry Moderated

9:30 - 11:00 am
LIFE FORM review and Discussion - NSF moderated

11:00 - 11:30 am
NSF Closed Session with Industry

11:30 - 12:00 pm
Summary & Closing Remarks
(Profs. Dave Martin, Greg Beaucage, Nick Kotov)

ADJOURN

Copies of Letters of Interest
Center for Hierarchical Emergent Materials (CHEM)

Potential Members:

<u>Letter Attached (20)</u>

Solvay
W. L. Gore & Associates
Procter & Gamble (Diaper Division)
Merck
Sumitomo Rubber Industries
The Chemours Company
The Shepherd Color Company
Mirexus Biotechnologies Inc.
Avery Dennison
Sun Chemical
Procter & Gamble (Corporate Functions R&D)
Bridgestone Americas Inc.
Air Force Research Laboratory (Emergent Materials)
Dupont, Biomaterial
Oak Ridge National Laboratory
Argonne National Laboratory
Air Force Research Laboratory (Structural Materials Division, Composites Branch)
PPG
Omya Inc.
Heraeus Medical Components, LLC

<u>Expecting Letter (e-mail confirmation 9)</u>

Dow Chemical
Procter & Gamble (Beauty and Skincare Division)
LyondellBasell
Polyone
ExxonMobil
Momentive
Arlanxco
Ford
Moderna

<u>Awaiting Reply (11)</u>

Goodyear Tire and Rubber
Sherwin Williams
BASF
SABIC Americas
KaoCollins
Michaelman
Continental Tire
Michelin
Novartis
Evonik
Unilever
HP
Clariant
Celanese
Wacker Chemie
Dow Silicones
Goodrich Tire
Nova Chemicals
Ashland Chemicals
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June 5, 2019

Prof. David C. Martin
Associate Dean for Research and Entrepreneurship
College of Engineering
The University of Delaware
Newark, DE 19716

Dear David,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (IUCRC) Center for Hierarchical Emergent Materials (CHEM). The topic and proposed team are of interest to Solvay and we would be happy to explore the possibility of participation in the center at a planning meeting in the Fall at the University of Cincinnati if schedules permit.

Solvay is a multi-specialty chemical company, committed to developing chemistry that addresses key societal challenges. Solvay innovates and partners with customers in diverse global end markets. Our products and solutions are used in planes, automobiles, smart and medical devices, batteries, in mineral and oil extraction, among many other applications, with sustainability being a key focus of our product offering. Our light-weighting materials enhance cleaner mobility, our formulations optimize the use of natural resources and our performance chemicals improve air and water quality. Several of the proposed activities of the center align with our interest areas.

We look forward to learning more at the planning meeting.

Best regards,

Matthew Taylor
Solvay Corporate Research & Innovation
R&I Director, North America
Tel.: +1 (215) 781-6467
Email: matthew.taylor@solvay.com

SOLVAY USA Inc
350 George Patterson Boulevard
Bristol, PA 19007
+1 215-781-6001
www.solvay.com

June 4, 2019

Professor Darrin Ponchan
Materials Science and Engineering
University of Delaware
Newark DE 19716

Subject: *Center for Hierarchical Emergent Materials (CHEM)*

Dear Darrin,

Thank you for sharing the information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) *Center for Hierarchical Emergent Materials (CHEM)*. The topic and proposed team are of interest to W. L. Gore & Associates and we would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Vivek Agarwal

W. L. Gore & Associates, Inc.
Core Tech
501 Vieves Way
Elkton, MD, 21922
Tel 302 506-3839
gore.com

The Procter & Gamble Company
Beckett Ridge Technical Center
8611 Beckett Road
West Chester, OH 45069

May 23, 2019

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are highly relevant to the areas of R&D for Procter & Gamble and I would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Dr. Michael Satkowski
Section Head
satkowski.mm@pg.com

June 6, 2019

To: Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

FROM: Matthew Lamm

SUBJECT: Center for Hierarchical Emergent Materials (CHEM).

Dear Professor Beaucage,

I have learned of the proposed NSF Industry and University Cooperative Research Center focusing on Emergent Hierarchical Materials (CHEM) from Professor Darrin Pochan. The proposed topics are of potential interest to Merck particularly in the areas of Pharmaceutical Sciences. We would like to learn more about the research thrusts of this center and will plan to attend the exploratory meeting this fall. Please inform us when the timing of the meeting has been finalized so we can plan accordingly.

Regards,

Matthew S. Lamm, Ph.D.
Director, Preformulation

Merck Research Laboratories
Merck & Co., Inc.

RY-80T-A128
126 East Lincoln Avenue
Rahway, NJ 07065
email: matthew.lamm@merck.com
phone: 732-594-5035

Sumitomo Rubber Industries, Ltd.
Kobe 651-0071, Japan

June 03, 2019

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Prof. Beaucage ,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are of interest, especially with respect to non-linear dynamic mechanical property of rubber vulcanizates consists of hierarchical structures such as inhomogeneous and homogeneous crosslinking network and filler particles. We would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Dr. Toshio Tada
Manager Material department III
t-tada.cx@srigroup.co.jp

Chemours™

The Chemours Company
1007 Market Street
PO Box 2047
Wilmington, DE 19899

302-683-8419t
chemours.com

June 06, 2019

Prof. David C. Martin
Associate Dean for Research and Entrepreneurship
College of Engineering
The University of Delaware
Newark, DE 19716

Dear David,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (IUCRC) Center for Hierarchical Emergent Materials (CHEM). The control of structure within particle systems is essential for the many applications of our current and future products. While this topic has been touched on in several instances in the past, there remains a general lack of robust scientific principles that can be applied generally to industrial systems where complex and competing multi-body interactions are prevalent. Scientific advances that help facilitate the control of hierarchical structure and designed performance in these systems is of significant interest to the Chemours Company. Recently, Chemours has engaged in collaborative research with several faculty members at the University of Delaware that are identified in the IUCRC proposal due to their unique capabilities and experiences in this area. We believe that advancing the science and building the future workforce in this topical area is likely to have a broad positive impact across chemical and manufacturing industries.

We appreciate you bringing this to our attention and would be happy to further explore the possibility of participation in the center at a planning meeting in the Fall at the University of Cincinnati.

Best regards,

Scott C. Brown, Ph.D.
Principal Scientist

Titanium Technologies
Research & Development
scott.c.brown@chemours.com
(302) 683-8419

The Shepherd Color Company

We Brighten Lives

June 6, 2019

Professor Gregory Beaucage
Professor of Materials Science and Engineering
492 Rhodes Hall
Department of Biomedical, Chemical, and Environmental Engineering
University of Cincinnati
Cincinnati, Ohio 45221-0012

Dear Professor Beaucage:

I was interested to learn of your efforts to organize a National Science Foundation (NSF) Center to study hierarchical materials. As you know, Shepherd Color is a local manufacturer of colored inorganic pigments and so understanding the nuances of the structure of our products (not only crystalline structure, but crystallite structure, particle size distribution, agglomerate structure, and dispersion and structure in use) is valuable to us. The capabilities of this center, both instrumental and research, may be of use to us.

You suggest there may be a meeting in the fall to allow the academic participants to meet with potential industrial partners to present the capabilities and suggest research areas. Please keep me informed about that meeting because we would be excited to attend the meeting and learn more about this NSF center.

Kind regards,

Geoffrey T. Peake

Geoffrey T. Peake
R&D Manager

4539 Dues Drive • Cincinnati, OH 45246 • Phone: (513) 874-0714 • Fax: (513) 874-5061 • www.shepherdcolor.com

June 3, 2019

Prof. Jonathan D. Nickels
Department of Chemical and Environmental Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Jon,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM)*****.** The topic and proposed team are of interest to Mirexuss and we would be happy to explore participation in the center at a meeting in the fall at the University of Cincinnati.   We will send a representative to this meeting.

Sincerely,

Phil Whiting, PhD
President & CEO
Mirexus Biotechnologies Inc.
574 Hanlon Creek Boulevard
Guelph, Ontario CANADA
N1C 0A1
Office (519) 829 1221 ext 201
Cell (905) 339 9907
www.mirexusbiotech.com

Reflective Solutions
7542 North Natchez Ave
Niles, IL 60714

Confidential

Date: May 28th, 2019

To,

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) Center for Hierarchical Emergent Materials (CHEM). The topics and proposed team are of interest to Avery Dennison across multiple divisions and we would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best Regards,

Nikhil Agashe, PhD
Global R&D Director
Avery Dennison, Reflective and Digital Ink Solutions

SunChemical®
a member of the DIC group DIC

Russell Schwartz
Chief Technology Officer
Sun Chemical Corporation
35 Waterview Boulevard,
Parsippany, NJ 07054 USA
Russell.Schwartz@sunchemical.com
T +1 973 404 6175
F +1 973 404 6807

May 28, 2019

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are of interest to Sun Chemical and we would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Sincerely,

Russell Schwartz

Procter & Gamble
Mason Business Center
8700 Mason Montgomery Road
Mason, Ohio 45040

May 24, 2019

Dr. Yoonjee Park
Department of Chemical and Environmental Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Dr. Park,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are broadly of interest to Proctor & Gamble, and several P&G representatives would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Dr. Ron Swift
Director, Corporate Functions R&D
The Procter & Gamble Company

BRIDGESTONE

Bridgestone Americas, Inc.
6533 South Mountain Road
Mesa, Arizona 85212
Phone: (480) 270-8251
Fax: (480) 270-2863

June 11, 2019

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) Center for Hierarchical Emergent Materials (CHEM). The topic, team and proposed focus are both interesting and relavent to Bridgestone's industrial activities. We would be happy to discuss participation in the center at a meeting in the Fall at the University of Cincinnati.

Sincerely,

William S. Niaura
Director - Innovation

Bridgestone Americas Inc.
6533 S. Mountain Rd
Mesa, AZ 85212

E-mail: NiauraWilliam@BFUSA.com
Phone: 480.270.8244
Cell: 615.557.3679 (preferred)

DEPARTMENT OF THE AIR FORCE
AIR FORCE RESEARCH LABORATORY
WRIGHT-PATTERSON AIR FORCE BASE OHIO 45433

5 June 2019

Air Force Research Laboratory
2179 12th St, AFRL/RX
Wright-Patterson AFB, OH 45433-7750

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) Center for Hierarchical Emergent Materials (CHEM). The topic and proposed team are of interest to the Air Force Research Laboratory and its Materials and Manufacturing Directorate, and we would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Dr. Richard A. Vaia
Senior Technologist, Emergent Materials
Air Force Research Laboratory
richard.vaia@us.af.mil

DuPont
Experimental Station
200 Powder Mill Road
Wilmington, DE 19806

May 20, 2019

Prof. David C. Martin
Associate Dean for Research and Entrepreneurship
College of Engineering
The University of Delaware
Newark, DE 19716

Dear David,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (IUCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The Biomaterial business unit in DuPont has already greatly benefited from the collaborations we have with University of Delaware (Prof. Arthi Jayaraman, Prof. Darrin Pochan, Prof. Norman Wagner). We are continuously looking for more opportunities to further strengthen our relationship with University Research Labs.

The topic and proposed team are of interest to DuPont and we would be happy to explore the possibility of participation in the center at a planning meeting in the Fall at the University of Cincinnati.

Best regards,

Kyle Kim, Ph.D.
Product Development Engineer
DuPont, Biomaterial
(302)-695-7374
kyle.kim@dupont.com

From: Urban, Volker S. urbanvs@ornl.gov
Subject: RE: Re: [EXTERNAL] Center for Emergent Hierarchical Materials
Date: June 9, 2019 at 1:59 AM
To: Gregory Beaucage gbeaucage@gmail.com

VU

Hi Greg,
Glad you sent a follow up – looks like I missed your earlier email last Sunday. Sorry about that!
Yes, certainly count me in; this sounds very exciting – soft matter is an area that we absolutely want to grow at SNS/HFIR, and growing our external user community is absolutely essential for that!
Are you saying that you need 9 letters from people at Oak Ridge? (9 per site) I may be able to make that happen – but you certainly will get one from me.
By when do you need it? Deadline?
Thanks!
Volker

From: Gregory Beaucage <gbeaucage@gmail.com>
Sent: Saturday, June 8, 2019 10:37 AM
To: Urban, Volker S. <urbanvs@ornl.gov>
Subject: [EXTERNAL] Re: Center for Emergent Hierarchical Materials

Hi Volker,

I think that it might be useful for someone from Oak Ridge to attend the meeting in October at UC. There will be12 faculty from Michigan, Delaware, and Cincinnati talking about substantially the use of scattering to study soft matter. Also rheologists, cryoTEM, and people fabrication hierarchical structures. Neutrons plays a role in this. We will certainly be sending down proposals. Maybe Venky or someone could come. I've attached a draft of the planning meeting proposal.

I need to get 27 letters from people who are interested in coming to the meeting (not a commitment). But it needs to be on letterhead.

It would be pretty useful at this stage. We need 9 per site to indicate interest but only 3 to fund which we already have. The team is Darrin Pochan, Norm Wagner, Ron Larson, Me, Dave Martin, Arthi Jayaraman, Nick Kotov. Most of those are publishing in Science/Nature every year. I don't think you will be bored.

Best wishes,

Greg

Draft of the proposal for the meeting:

Jan Ilavsky, PhD
Scientist
USAXS instrument

X-ray science division
Advanced Photon Source
Argonne National Laboratory
9700 South Cass Avenue, Bldg. 433A
Argonne, IL 60439-4859

1-630-252-0866 phone
1-630-252-0460 fax
ilavsky@aps.anl.gov
http://usaxs.xray.aps.anl.gov

June 9, 2019

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information about the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are of interest to my own research at Advanced Photon Source, Argonne National Laboratory. Collaboration with the center and its industrial participants promises new and exciting science opportunities for our USAXS/SAXS/WAXS materials characterization facility. As you know, growth of our facility user community and widening of its impact on industrial research of US industry is of prime interest to me.

Therefore, I would like to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Jan Ilavsky

DEPARTMENT OF THE AIR FORCE
AIR FORCE RESEARCH LABORATORY
WRIGHT-PATTERSON AIR FORCE BASE OHIO

June 10, 2019

FROM: Hilmar Koerner, Jeffery Baur
Air Force Research Laboratory
Materials and Manufacturing Directorate
2941 Hobson Way
Wright-Patterson Air Force Base, OH 45433

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,
I am writing to you expressing our interest in your proposed NSF Industry & University Cooperative Research Center (I/UCRC) Center for Hierarchical Emergent Materials (CHEM). Particular topics, including neutron and x-ray scattering, rheology, synthetic expertise and coarse grain simulation of complex structures are very relevant to our strategy and vision within two research teams in the Composites Branch of the Strucutal Materials Division (Polymer Matrix Composites Materials and Processes – Hilmar Koerner; Composite Performance – Jeffery Baur). Specifically, emerging manufacturing processes for continuously and discontinuously filled matrix composites require a whole new set of advanced characterization and modeling approaches that your Center is addressing. The impacts of hierarchical structure in additive manufacturing and traditionally processed composites on performance are our primary interest. We are eager to explore participation during your Fall meeting at the University of Cincinnati.

Sincerely,

Hilmar Koerner

Jeffery Baur

Monroeville Business & Technology Center
440 College Park Drive
Monroeville, PA 15146-1536 USA
Mobile: (412) 605-4760
E-Mail: nsilvernail@ppg.com
Web: www.ppg.com
www.ppgsilica.com

Nathan Silvernail
Silica Research Manager

June 10, 2019

Prof. Gregory Beaucage
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati OH 45221-0012

Dear Greg,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (I/UCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are of interest to PPG and we would be happy to explore participation in the center at a meeting in the Fall at the University of Cincinnati.

Best regards,

Omya Inc.
9987 Carver Road
Suite 300
Cincinnati, Ohio 45242
U.S.A.

Tel +1-513-387-4600
Tel +1-800-749-6692
Fax +1-513-387-4692

www.omya-na.com

Omya Inc.
Cincinnati, OH

June 10, 2019

Gregory Beaucage, Ph.D.
Department of Chemical and Materials Engineering
University of Cincinnati
Cincinnati, OH 45221-0012

Dear Greg,

Thank you for sharing information about the proposed ***Center for Hierarchical Emergent Materials (CHEM)*** through the NSF Industry-University Cooperative Research Centers (IUCRC) program. The proposed team's expertise and the research topics are of interest to Omya and we would be glad to explore participation in the research center at a meeting at the University of Cincinnati in the Fall.

Sincerely,

Andrew Mulderig, Ph.D.
Scientist
Andrew.Mulderig@omya.com

Heraeus

May 20, 2019

Prof. David C. Martin
Associate Dean for Research and Entrepreneurship
College of Engineering
The University of Delaware
Newark, DE 19716

Dear David,

Thank you for sharing information concerning the proposed NSF Industry & University Cooperative Research Center (IUCRC) ***Center for Hierarchical Emergent Materials (CHEM).*** The topic and proposed team are of interest to Heraeus Medical Components and we would be happy to explore the possibility of participation in the center at a planning meeting in the Fall at the University of Cincinnati.

Best regards,

Jeffrey Hendricks, PhD
Vice President Business Development
Heraeus Medical Components, LLC
5030 Centerville Rd.
St. Paul, MN 55127
jeffrey.hendricks@heraeus.com