COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./CLOSING DATE/if not in response to a program announcement/solicitation enter NSF 11-1

NSF 10-595 **03/06/11**

FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)

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NSF PROPOSAL NUMBER

1134832

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316000989

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NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE

University of Cincinnati Main Campus

AWARDEE ORGANIZATION CODE (IF KNOWN)

0031252000

ADDRESS OF AWARDEE ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE

University of Cincinnati Main Campus
University Hall, Suite 530
Cincinnati, OH. 452210222

NAME OF PRIMARY PLACE OF PERF

University of Cincinnati Main Campus

ADDRESS OF PRIMARY PLACE OF PERF, INCLUDING 9 DIGIT ZIP CODE

University of Cincinnati Main Campus
492 Rhodes Hall
Cincinnati ,OH ,452210012 ,US.

IS AWARDEE ORGANIZATION (Check All That Apply) (See GPG II.C For Definitions)
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TITLE OF PROPOSED PROJECT **Planning Grant: I/UCRC for The Center for Macromolecular Topology (CMT)**

REQUESTED AMOUNT	PROPOSED DURATION (1-60 MONTHS)	REQUESTED STARTING DATE	SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE
$ **14,500**	**12** months	**09/01/11**	

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☐ HISTORIC PLACES (GPG II.C.2.j)
☐ EAGER* (GPG II.D.2) ☐ RAPID** (GPG II.D.1)
☐ VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____
PHS Animal Welfare Assurance Number _____
☐ HUMAN SUBJECTS (GPG II.D.7) Human Subjects Assurance Number _____
Exemption Subsection _____ or IRB App. Date _____
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UK
☐ HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.G.1)

PI/PD DEPARTMENT
Materials and Chemical Engineering

PI/PD FAX NUMBER
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CO-PI/PD				
CO-PI/PD				
CO-PI/PD				

Electronic Signature

CERTIFICATION PAGE

Certification for Authorized Organizational Representative or Individual Applicant:

By signing and submitting this proposal, the Authorized Organizational Representative or Individual Applicant is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding debarment and suspension, drug-free workplace, lobbying activities (see below), responsible conduct of research, nondiscrimination, and flood hazard insurance (when applicable) as set forth in the NSF Proposal & Award Policies & Procedures Guide, Part I: the Grant Proposal Guide (GPG) (NSF 11-1). Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U. S. Code, Title 18, Section 1001).

Conflict of Interest Certification

In addition, if the applicant institution employs more than fifty persons, by electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative of the applicant institution is certifying that the institution has implemented a written and enforced conflict of interest policy that is consistent with the provisions of the NSF Proposal & Award Policies & Procedures Guide, Part II, Award & Administration Guide (AAG) Chapter IV.A; that to the best of his/her knowledge, all financial disclosures required by that conflict of interest policy have been made; and that all identified conflicts of interest will have been satisfactorily managed, reduced or eliminated prior to the institution's expenditure of any funds under the award, in accordance with the institution's conflict of interest policy. Conflicts which cannot be satisfactorily managed, reduced or eliminated must be disclosed to NSF.

Drug Free Work Place Certification

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant is providing the Drug Free Work Place Certification contained in Exhibit II-3 of the Grant Proposal Guide.

Debarment and Suspension Certification

(If answer "yes", please provide explanation.)

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency? Yes ☐ No ☒

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant is providing the Debarment and Suspension Certification contained in Exhibit II-4 of the Grant Proposal Guide.

Certification Regarding Lobbying

The following certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding $100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding $150,000.

Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:
(1) No federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any federal contract, the making of any Federal grant, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions.
(3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, Title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than $10,000 and not more than $100,000 for each such failure.

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Certification Regarding Flood Hazard Insurance

Two sections of the National Flood Insurance Act of 1968 (42 USC §4012a and §4106) bar Federal agencies from giving financial assistance for acquisition or construction purposes in any area identified by the Federal Emergency Management Agency (FEMA) as having special flood hazards unless the:
(1) community in which that area is located participates in the national flood insurance program; and
(2) building (and any related equipment) is covered by adequate flood insurance.

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Certification Regarding Responsible Conduct of Research (RCR)
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The undersigned shall require that the language of this certification be included in any award documents for all subawards at all tiers.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME **Mary Ucci**	**Electronic Signature**	**Mar 8 2011 7:50AM**

TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS	FAX NUMBER
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* EAGER - EArly-concept Grants for Exploratory Research
** RAPID - Grants for Rapid Response Research

COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

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NSF 10-595 **03/06/11**

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NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE

University of Michigan Ann Arbor

AWARDEE ORGANIZATION CODE (IF KNOWN)

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NAME OF PRIMARY PLACE OF PERF

University of Cincinnati Main Campus

ADDRESS OF PRIMARY PLACE OF PERF, INCLUDING 9 DIGIT ZIP CODE

University of Cincinnati Main Campus
492 Rhodes Hall
Cincinnati ,OH ,452210012 ,US.

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UK
☐ HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.G.1)

PI/PD DEPARTMENT
Chemical Engineering

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Electronic Signature

CERTIFICATION PAGE

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(2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions.
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The undersigned shall require that the language of this certification be included in any award documents for all subawards at all tiers.

AUTHORIZED ORGANIZATIONAL REPRESENTATIVE	SIGNATURE	DATE
NAME **Marvin Parnes**	**Electronic Signature**	**Mar 7 2011 11:30AM**

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* EAGER - EArly-concept Grants for Exploratory Research
** RAPID - Grants for Rapid Response Research

Planning Grant: I/UCRC for The Center for Macromolecular Topology (CMT)

Intellectual Merit of the Center: The Center for Macromolecular Topology (CMT) will address the need in the polymer industry to synthetically control, characterize, model and simulate complex macromolecular architectures to manipulate mechanical and rheological properties. This topic has broad industrial and academic interest making it ideal for an I/UCRC Center. Control and quantification of complex macromolecular architectures is of pivotal importance in the polyolefin industry where the addition of one long chain branch per ten thousand carbon atoms in polyethylene can increase the viscosity by a factor of 35. Often the source of trace amounts of long chain branching is difficult to determine and characterization is challenging. Similarly, control of branching in gels, networks and elastomers remains a synthetic and characterization challenge of broad importance to industry. Complex macromolecular topologies are also of importance to model polymeric systems that are targeted for new technologies such as molecular machines. Some of these synthetic systems serve as simple representatives of molecular characteristics displayed by biological molecules. The two PI's offer complementary skill sets of interest to industry focusing on characterization and rheology. The two universities can also offer expertise in synthesis, modeling and simulation. Interactions with other universities and international centers, particularly the Polymer IRC at the University of Leeds, are planned. The Leeds center differs from CMT in that it focuses on simulation and modeling of complex topologies while the CMT will focus on characterization and rheology. Ron Larson, already has strong interactions with the Leeds Center.

One initial focus of the center will be on control of molecular topology in polyethylene. Both the Michigan and Cincinnati groups have active research programs in this area that have significant industrial interaction. Currently, work in understanding structure/property relationships in branched polyolefins is duplicated at a number of industrial research labs. CMT can serve as a hub for pooling of non-proprietary information and to set standards for the description of complex molecular topologies especially in polydisperse systems of industrial importance. Manufacturers of polyolefins such as Dow, LondellBasell and ExxonMobil have expressed a strong interest in the proposed center. The topic of molecular topology is also of interest to industries involved in gels, elastomers and hyperbranched structures such as P&G, Bridgestone/Firestone and DSM. National laboratory participation in the center will involve characterization techniques involving neutron scattering (ORNL) and interest in utilization of these materials in weapons systems and other high technology areas (Sandia Natoinal Lab, Air Force Research Laboratory).

Broader Impact of the Center: The CMT will develop human capacity in the chemical industry. The center will significantly enhance the nation's research infrastructure base, which is losing ground to European, Asian and Middle Eastern competition in the polyolefin and other industries targeted by the center. The center will coordinate internet based video courses on rheology, scattering, synthesis and modeling of complex macromolecular systems that will be available to industrial as well as academic participants and the general public on arrangement with the Universities. CMT will actively recruit women and minority graduate and undergraduate students.

The center has as a main goal enhancement of the intellectual capacity of the engineering workforce and capabilities in controlling molecular topology. Improvement in our control of molecular topology will lead directly to improvements in a wide range of consumer and industrial products from gels to tires; from plastic packaging to viscosity enhancement in oils.

TABLE OF CONTENTS

For font size and page formatting specifications, see GPG section II.B.2.

*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.

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*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 Macromolecular Topology (CMT). The grant will support a meeting organized by the University PI's at the University of Michigan and at the University of 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, the organization and the types of memberships/affiliations in the Center.

Strategy: The CMT will be developed in collaboration with the 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 2011 at the University of Cincinnati. The strategy for implementing the objectives will be to present a basic format for the center and several other formats based on a Center in the UK and ideas proposed by industrial and national lab participants. The Center 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: The potential members of the Center's two sites are listed below: (*** & bold = letter of interest provided;** only * = verbal/e-mail statement of interest)

University of Cincinnati

***Procter & Gamble, Phase & Colloid Science Analytic Division (First Membership)**
***LyondelBasell Industries**
***Dupont, Experimental Station, Wilmington, DE**
***Oak Ridge National Laboratory**
***Bridgestone/Firestone**
***Eclipse Film Technologies**
***ThreeBond Corporation**
*Avery Dennison Corporation
*SABIC Americas
DSM Hybrane Division
Goodyear Tire & Rubber
Goodrich Tire
PPG Industries
Nova Chemicals
Ashland Chemicals
Ticona Coporation
PolyOne Corporation

University of Michigan

***ExxonMobil, Baytown, TX (First Membership)**
***Dow Chemical, Freeport TX**
***Air Force Research Laboratory**
***Procter & Gamble Materials Science & Technology (Second Membership)**
***Myaterials**
***Dow Corning Corporation**
*ExxonMobil, Research & Engineering Co. (Second Membership)
*Procter & Gamble, Baby Care Division (Third Membership)
*Sandia National Laboratory
Michigan Molecular Institute
3M Corporation
Soldier Research, Development and Engineering Center (NSRDEC) U. S. Army Natick, MA
Total Petrochemicals
ChevronPhillips

Meeting Planning:

Location: University of Cincinnati, Kingsgate Conference Center
Date: Fall, 2011

Meeting Format and Organization: A draft agenda for the planning meeting is shown in the Supplimental Documents section of this proposal. The meeting will open with brief remarks from the Vice President for Research at the University of Cincinnati and from a representative of the University of Michigan. These speakers will be introduced by the two 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 at the University of Cincinnati site. After Lunch, projects at the University of Michigan will be described. A booklet with one-page descriptions of possible projects form the two 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 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. 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 two 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:

Prof. Greg Beaucage & Prof. Ron Larson: 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.

Center Evaluator: 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.

NSF Representative: 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:

The polymer industry involves a wide range of companies and government facilities involved in the synthesis, processing and application of synthetic macromolecules. Understanding the structure/property relationships for these materials involves, to a large part, characterization and control over the chemical and stereo-chemical composition and the molecular weight distribution. However, two polymers of identical molecular weight, chemical and stereo-chemical structure can have completely different dynamic and static properties depending on the chain topology and branching. For example, a cyclic polymer, a star polymer, a long-chain branched and a linear chain each displays dramatically unique rheological behavior while presenting similar characterization fingerprints. Control, prediction and optimization of synthetic protocols depend on quantification of these topological differences. To make matters worse, commercial polymers are subject to a small amount of reactivity during processing that can lead to slight changes in the topology, for instance the occasional addition of a long chain branch in polyolefins by hydrogen abstraction, end group reactivity, cyclization in polysiloxanes, transesterification in polyesters, or vinyl reactivity in polystyrene. This imperceptible change in structure during processing can have dramatic effects on rheology. The addition of one long chain branch per 10,000 carbons in polyethylene can result in a 35 times increase in the zero shear rate melt viscosity. Changes in chain topology can have an unpredictable impact on other properties of polymers in various applications.

In addition to commodity polymers, many segments of the polymer industry focus on controlled macromolecular topology for functional materials. Chief in this arena is the elastomer and rubber industry but parallel interests lie in the manufacture and use of gels in a wide range of applications. Recently materials that bridge weakly branched and crosslinked systems have been developed. These hyperbranched and dendritic materials offer unique properties for a wide range of specialty applications such as drug delivery, absorption, and enhancement of rheology. Control over structure/property relationships, quantification of complex topological structure and understanding the structural basis for rheological and dynamic mechanical properties are vital to improvement of products and understanding industrial problems in synthesis, processing and use of these materials.

The proposed center seeks to apply new analytic tools, synthetic capabilities and molecular modeling to control and understand macromolecular materials of complex topology. The two PI's are pioneers in the application of rheological and scattering techniques to this problem and have recently made advances that may serve to revolutionize our understanding of macromolecular topology. Ron Larson has also used new chromatographic techniques to segregate chains of variable branch content. The PI's have teamed with other experts at the University of Michigan and at the University of Cincinnati to provide a rounded team effort that can contribute to this important area of polymer and materials science. The CMT also plans to

work with researchers at other institutions in the US and in Europe to expand the center's capability in keeping with the needs of its industrial and national laboratory partners.

The center plans to link university, industry, and national lab resources to leverage research efforts, facilities and expertise. For example, for long chain branching in polyolefins the main interest is in the rheological consequences of chain topology, however, detailed mappings of the chain structure, especially for commercial resins, is not possible using commonly used methods such as fractionation followed by light scattering, dilute solution viscosity and other analytic methods. Key features such as the branch-on-branch structure or the branch length cannot be quantified even with these elaborate techniques. Without this structural information it is difficult to develop a comprehensive structural model to predict rheology. Further, chemical mechanisms associated with the formation of branched structures can only be guessed at with the current state of quantification of chain structure. So a team effort coupling catalytic chemists, rheologists, molecular morphologists, simulators and modelers is needed. For neutron scattering analytic techniques, the center can coordinate neutron beam time requests with instrumental scientists at Oak Ridge National Lab. Oak Ridge can also provide model branched polymers through the Center for Nano-Materials Science (CNMS) which has a unique user focused synthetic capability. For the SANS studies, the CMT Center can organize the research team as well as provide logistical support to develop this project. The Center can also provide training through short courses in techniques used in the research effort as well as to provide a forum between catalyst development companies, polyolefin producers, polymer film processing companies and polyolefin end users such as P&G, facilitating targeted research and development work. Similar teams can be assembled from Center participants for gels, elastomers, hyperbranched polymers and other areas. The Center will provide interaction between these research areas through emphasis on overlap across research areas. There is a great potential for synergy between the different commercial areas impacted by macromolecular topology. For example, understanding of the rheology of long chain branched polyolefins could be put to bear on problems during curing of elastomers in the manufacture of tires.

Existing Capabilities and Expertise:

University of Cincinnati: Beaucage's research effort at the University of Cincinnati will involve a novel characterization method using small-angle neutron scattering developed at UC over the past 6 years that allows for the quantification of macromolecular topology using milligrams of sample for commercial or model materials [1-9]. The scaling method allows for the determination of molar branch fraction, ϕ_{Br}, average number of branches, n_{Br}, number of short chain branches, n_{SCB}, number of inner segments or branch-on-branch segments, n_i, the average branch length, z_{Br}, and the fractional steric interaction, ϕ_{si} [9]. Figure 1 [8] shows results from a commercial LLDPE sample that was separated according to branch content using temperature rising elution fractionation. Oak Ridge National Laboratory will team with Beaucage in this research. Beaucage also has extensive in-house x-ray and light scattering facilities that may be used for some aspects of the Center research.

Beaucage has also worked extensively with rubber manufactures such as Goodyear and Dow Corning, mostly in the use of x-ray scattering to characterize reinforcing materials [10-12]. Beaucage also has developed the only comprehensive structural model for polymer gels that can couple mechanical behavior with the structure observed in neutron scattering measurements. This work is currently being conducted in collaboration with Procter & Gamble Corporation [13-14].

The University of Cincinnati also has a number of other faculty who will likely participate in the Center including Prof. Stephen Clarson who is an expert at polysiloxane chemistry and silicone elastomers and has strong industrial contacts with the siloxane industry particularly Dow Corning, Prof. Jude Iroh who is an expert in epoxy chemistry and has worked with the Air Force Research Laboratory on the development of branched thermoset structures. Iroh also has extensive experience with polypyrrole chemistry; Asst. Prof. Vikram Kuppa who is an expert at modeling and simulation of complex macromolecular architectures and who has ties with Bridgestone/Firestone. The center will also expand to other faculty at UC through competitive calls for proposals.

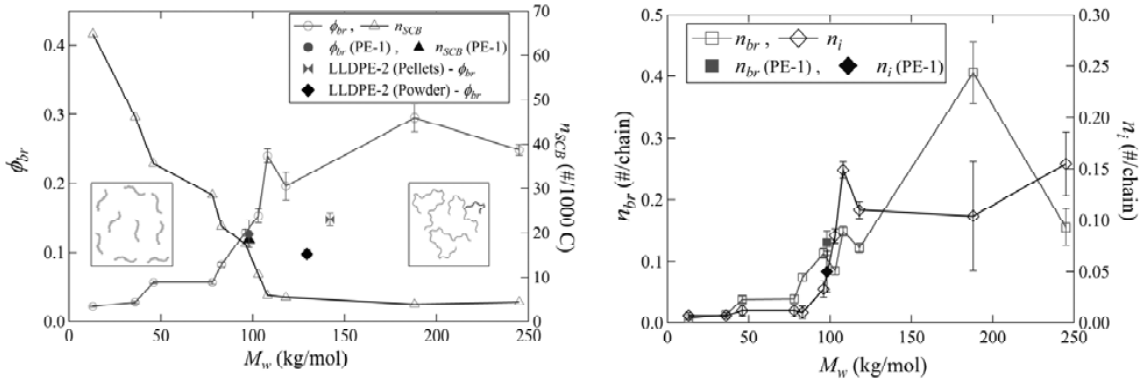


Figure 1. a) Plot of mole-fraction LCB content, ϕ_{br}, from equation (7) and number of SCBs per 1000 Carbon atoms, n_{SCB}, from NMR against the weight-average molecular weight, M_w, obtained from SANS [8]. b) Plot of number of LCB sites per chain, n_{br}, from equation (9) and number of inner segments per chain, n_i, versus M_w [8]. The filled data points represent the corresponding values obtained for PE-1 that was fractionated by TREF.

University of Michigan: Ron Larson is an expert in rheological characterization of polymers, especially as it pertains to complex topological structures such as occur in long-chain branched polyolefins. Larson has authored or co-authored three books: *Constitutive Equations for Polymer Melts and Solutions*, *The Structure and Rheology of Complex Fluids* [16] and *Structure and Rheology of Molten Polymers* [17], the latter, co-authored with John Dealy, having become a popular reference for the polyolefin industry in understanding the rheology of topologically complex macromolecules. Larson's recent work involves understanding the rheology of complex branched polymers that include asymmetric H-polymers that are produced at Oak Ridge National Laboratory in collaboration with Jimmy Mays and his associates, Figure 2b. Larson has developed software that can predict the dispersion of chain structure of polyethylene produced using single-site metallocene catalysts. The chain structure produced in Larson's simulation can be used in other software to calculate the low extension dynamic rheological response. Figure 2a shows such calculations for asymmetric H-polymers.

In addition to Larson a number of well known, as well as promising young macromolecular scientists are expected to participate in the Center at the University of Michigan site. Prof. Rick Laine is know for his work in sol-gel chemistry and inorganic and organometallic branched polymers. Laine has his own company as well as extensive industrial interactions. Prof. Peter Green is an expert at polymer physics and has worked with elastomer-based nano-composites. He has strong connections to the Department of Energy and Sandia National Laboratories. Prof. Mike Solomon, in the Chemical Engineering Department, is interested in working on supramolecular structures such as the formation of fibrillar structures in

polymers under shear flow. Mike has received funding from Procter & Gamble for his work in colloidal gellation.

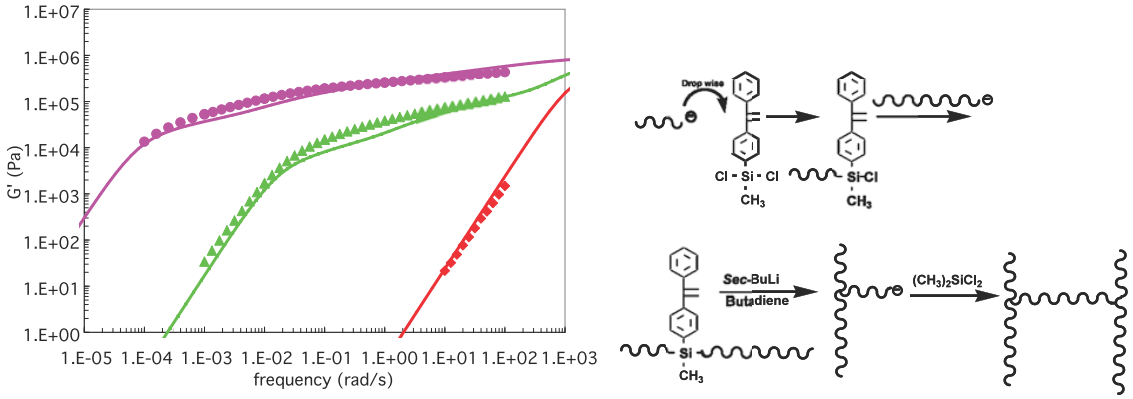
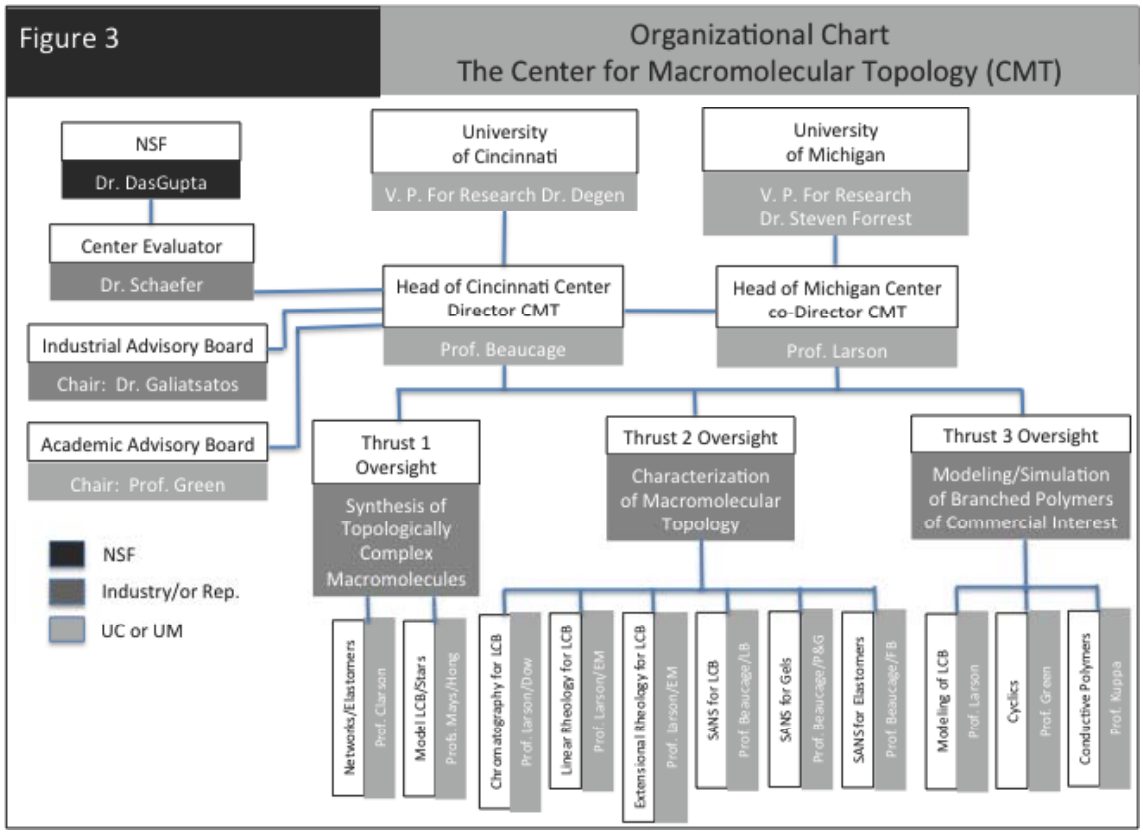


Figure 2. (a) Storage modulus of "H" polymer (violet), linear-shaped (red), and a 50-50 blend (green), all of polybutadiene. Lines are calculations based on Larson's hierarchical model and points are experimental measurements. (b) An example of a synthetic scheme for making monodisperse asymmetric H-PBd in the Mays lab.

Center's Structure:



Diversity Plan:

The CMT will actively recruit minorities and women to participate in the center research efforts. Several of the expected participating members are African American (Peter Green and Jude

Iroh). The center will request REU and RET funding that will specifically target the participation of minority and women undergraduates and high school teachers in the Center's research.

Proposed Projects:

Six of the possible projects that would be pursued by the Center are discussed below. During the planning meeting a larger number of specific projects will be discussed in oral presentations and posters. A booklet of one-page project descriptions will be distributed.

University of Cincinnati

1) Branched Structure of Chrome Resins and Rheological Consequences
2) Macromolecular Structure of Gels
3) Network Structure of Conductive Polymers for Photovoltaic Devices

University of Michigan

4) Model Polybutadiene, and Polyethylene for Structure/Rheology Relationships.
5) Software Development for Interpretation of Rheological Data
6) Sol-Gel Chemistry for Photovoltaics

1) Branched Structure of Chrome Resins and Rheological Consequences

Proposed Team: G. Beaucage; R. Larson, LyondellBasell, Total, ExxonMobil, Dow.

Project Objectives: Chromium oxide is one of the earliest catalysts for the synthesis of polyethylene having been patented in 1951 [16]. While chrome resins are widely produced, an understanding of the branching structure has remained elusive with contradictory results from different techniques. Part of the confusion over the structure of chrome resins lies in the variability of branch content and hyperbranched content depending on the specific reaction scheme. A further complication lies in the terminal vinyl groups that can react in processing and lead to more complicated molecular topologies as a function of processing conditions. We propose a comprehensive study of the structure/property relationships for a series of commercial chrome resins with the goal of determining the nature of the branched structure, the source of branching and the consequences on the linear and extensional rheology in these systems. The goal of the research is to develop general predictive capabilities as well as fundamental understanding of the nature of chrome resins. The polyethylene samples for this study will be guided by industrial interaction with the project.

Industrial Relevance: The chrome resin project focuses on a longstanding issue in the polyolefin industry and seeks to resolve a fundamental gap in our understanding of these widely used commercial materials.

Center Relevance: This project addresses a commercially relevant problem involving macromolecular topology so it fits well within the intent of the Center.

Experimental Plan: Chrome resin samples will be obtained from industrial partners after a discussion with the project team. Samples will be prepared for rheological and neutron scattering measurements. Existing data from corporate sponsors will be pooled with the new characterization methods to develop a comprehensive understanding of structure in these resins.

Milestones and Time to Completion: The project will involve quarterly 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. Rheological experiments will follow approximately the same schedule. After the first year we expect to have preliminary analysis on a series of 10 chrome resins sufficient for understanding the fundamental structural range in these macromolecules. In the second year we intend to investigate the role of processing on the development of branching in the chrome resins, using the first year results to select likely

materials for understanding structural change in processing. 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 of the results from the first two 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 $55,000 per student so a total of $110,000 per year involving two center memberships, total cost of $330,000.

First Year Deliverables: Structural description of 10 chrome resins; rheological calculations based on this structural information and; experiments to verify these calculations.

End of Project Deliverables: The project will result in at least one publication dealing with structure/property relationships in chrome resins that will be aimed at resolving debates concerning the structure of chrome resins. The final report will describe methods to control structure so as to manipulate properties in chrome resins.

2) Macromolecular Structure of Gels

Proposed Team: G. Beaucage; Procter & Gamble, Oak Ridge National Lab.

Project Objectives: Polymer gels are widely used in absorbants, delivery devices, structural elements of devices and a wide range of other uses. Despite the wide range of uses and history of importance of gels, the structure which can be observed by small-angle neutron scattering (SANS) bears little resemblance to the structure proposed in the two prominent models, Flory-Rehner Theory and the de Gennes blob model. Recently Sukumaran and Beaucage have proposed a new model called the Gel Tensile-Blob (GTB) Model that can predict swelling properties and quantify the network mesh size based on SANS data [10,11]. We propose to study poly(sodium acrylate) superabsorbent hydrogels using SANS and the GTB model to quantify the network mesh size as a function of network forming reaction conditions. The result of this study will be a demonstration of the viability of the GTB model for polyelectrolyte networks and a fundamental understanding of the relationship between the network structure, synthetic conditions and swelling and mechanical properties of gels.

Industrial Relevance: The superabsorbent gels are use by P&G in the manufacture of diapers and other consumer products. These materials are also use in agricultural and biomedical applications across a wide range of fields.

Center Relevance: This project addresses a commercially relevant problem involving macromolecular topology so it fits well within the intent of the Center.

Experimental Plan: Superabsorbant samples, provided by Procter & Gamble, will be swollen in D_2O to enhance neutron contrast. Figure 7a shows preliminary data from a swollen superabsorbent sample as well as the GTB fit to the data.

Milestones and Time to Completion: The project will involve quarterly 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. After the first year we expect to have preliminary analysis on a series of 10 superabsorbant gels sufficient for understanding the fundamental structural features of PAA networks. In the second year we intend to investigate variable synthetic conditions including network formation from the melt versus from solution and at various concentrations near the overlap concentration to manipulate chain entanglement. 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 a graduate student at the University of Cincinnati. The approximate cost per year will be $55,000 per year, total cost of $165,000.

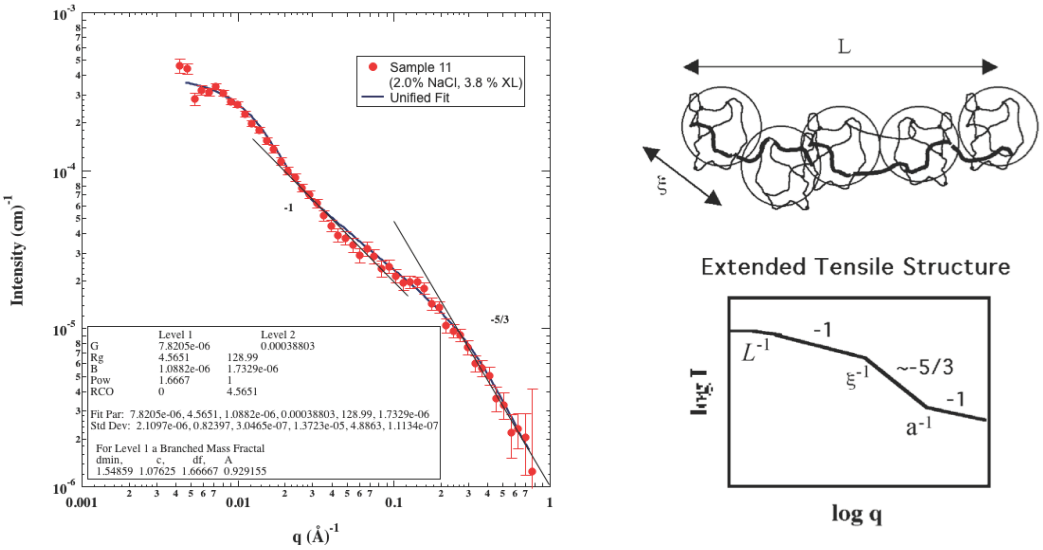


Figure 7. (a) Preliminary data from ORNL/HFIR facility on a PAA gel with 3.8 % cross linker concentration and swollen in a 2% salt solution. The fit is to the GTB model and reflects a mesh size of 44.7 nm with a tensile structural transition at 2.1 nm. The data also contains information concerning the network topology that reflects details of the gel structure. [18] (b) Schematic of the GTB model from [14].

First Year Deliverables: Structural description of 10 superabsorbent gels and correlation with synthetic conditions.

End of Project Deliverables: The project will result in at least one publication dealing with structure/property relationships in superabsorbent gels aimed at resolving debates concerning the structure of superabsorbent gels and to develop relationships between synthetic conditions and gel structure/mechanical properties and swelling behavior. The final report will describe methods to control structure so as to manipulate properties in superabsorbent gels.

3) Network Structure of Conductive Polymers for Photovoltaic Devices

Proposed Team: J. Iroh, V. Kuppa, AFRL, Sandia National Lab.

Project Objectives: Conductive polymers have been widely proposed as components of photovoltaic devices. In many cases conductive polymers are intractable so that description of the molecular structure has been impossible. One possibility is to use computer simulations of reaction conditions to predict structures and properties and to compare properties from these simulated structures with those of measured properties on real photovoltaic layers. This project proposes to couple synthetic expertise of Prof. Iroh at the University of Cincinnati with the simulation and modeling expertise of Prof. Kuppa to develop an understanding of the structure of conducting polymer layers through comparison of experimentally produced polypyrrole films to properties of simulated molecular topologies.

Industrial Relevance: Production of photovoltaic devices using conducting polymers is a promising technology for military and commercial applications. The lack of understanding of molecular structure for conducting polymer layers has hindered progress in this technology.

Center Relevance: This project addresses a commercially relevant problem involving macromolecular topology since it is believed that polypyrrole films display a ramified molecular structure.

Experimental Plan: The project will require one graduate student working between the two groups on computer simulations and on synthesis. It is expected that the students will use his dual experience to guide the simulations by experimental reality and will target measurable properties such as conductivity and IR spectra from these films through his experimental experience.

Milestones and Time to Completion: The project will involve weekly meetings of the project participants. The project will focus on simple synthetic schemes that can be easily modeled. The first year will result in preliminary results to assess the viability of the project. In the second year it may be necessary to expand the project to two students if the first year results warrant further study. The second year will focus experimental and modeling/simulation work on the most viable systems guided by the first year studies. 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 guided by review by the funding agencies of the results from the first two years.

Annual and Total Cost to Completion: The project will require a graduate student at the University of Cincinnati. The approximate cost per year will be $55,000 so a total of $165,000 involving one center membership.

First Year Deliverables: Preliminary assessment of the approach to understand the structure of polypyrrole films for photovoltaic devices.

End of Project Deliverables: The project will resolve some of the structural complexities of conducting polymer films and will result in several publications in this area that can be used to guide synthesis of photovoltaic devices. The final report will describe methods to control structure so as to manipulate properties in polypyrrole films and other conducting polymers.

4) Model Polybutadiene and Hydrogenated PBD for Structure/Rheology Relationships.

Proposed Team: R. Larson, G. Beaucage, J. Mays/K. Hong ORNL, ExxonMobil.

Project Objectives: Rheological modeling of branched macromolecular structures involves consideration of the hierarchy of structure present in a topologically complex molecule. A sort of triage is performed on the structure to ascertain levels of the structure that will be considered in sequence in terms of molecular relaxation. For instance, the short arms relax first and a relaxation time is calculated for these and then used to determine the relaxation of the main chain using a bead and string type model. This method works well in predicting the linear viscoelastic response of many complex macromolecular topologies especially for model structures such as monodisperse H-polymers mentioned above. The proposed work seeks to couple this hierarchical approach to rheology with new analytic methods using neutron scattering with the goal of using average structural parameterization in terms of branch length, number of branches, and number of inner segments (branch-on-branch structure) to calculate the rheological performance of commercial polymers composed of a blend of complex topological structures. There are two main approaches, first, the SANS model can be used to populate a distribution of chains that can be introduced to existing programs for calculation of the dynamic viscosity. Second, the average parameters obtained from SANS could be used directly to calculate the rheology by using a simple average structural model directly related to the parameterization of the distribution by scattering. Branching structures and molecular weight distributions will also be assessed by thermal gradient interaction chromatography (TGIC) by the Mays group.

Industrial Relevance: The proposed work seeks to advance existing rheological calculations to use new statistical information in order to predict the rheological performance of commercial polymers. If this process is successful it will lead to a deeper understanding of the molecular structure/rheological property relationships for topologically complex macromolecules.

Center Relevance: This project addresses a commercially relevant problem involving macromolecular topology so it fits well within the intent of the Center.

Experimental Plan: Model branched and linear polymer samples will be synthesized at the Center for Nanophase Materials Science (CNMS) at Oak Ridge National Lab (ORNL). These monodisperse materials, and blends with linear and other branched structures, well be measured using SANS at the High Flux Isotope Reactor (HFIR) at ORNL and the quantified structural parameters will be used in the two methods mentioned above to calculate the viscoelastic properties. Predictions will be compared with rheological measurements on the same samples and blends.

Milestones and Time to Completion: During the first year the project will explore relatively simple structures such as symmetric and asymmetric star polymers and blends with linear polymers. These systems are similar to some metallocene resins. Comparison with Metallocene resins will be made. With success in the first year further studies of H-polymers of variable arm length distribution will be considered and blends with stars and linear polymers. For all samples and blends SANS and dynamic rheology measurements will be performed.

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 $55,000 per student so a total of $110,000 per year involving two center memberships, total cost of $330,000.

First Year Deliverables: Initial studies of star polymers and blends. At the end of the first year demonstration of concept will be made and the first paper will be in the process of submission.

End of Project Deliverables: The project will result in a number of publications describing methods to use SANS data to calculate rheological properties. The final report will describe methods to control structure so as to manipulate properties in branched polyolefins.

5) Software Development for Interpretation of Rheological Data

Proposed Team: R. Larson, Dow Chemical.

Project Objectives: Calculation of the dynamic rheological properties for macromolecular systems of complex topology is currently possible using several computer routines developed by Prof. Larson and other researchers. These tools are now used in industry to predict the expected rheological consequences of various catalyst manipulations. Several areas remain to be developed in extending this suite of programs. The current software tools are limited to linear rheology at low extension for fairly simple structural models. For example is it not possible to model the rheological response of dendrimers, hyperbranched chains or cyclics using these models. Further, the current software does not allow calculation of extensional viscoelastic response. We propose to address the issue of chain molecules of higher complexity and to develop tools to predict the extensional viscosity using the hierarchical approach discussed above. We also plan to integrate the software into the popular IRIS package for interpretation of rheological data.

Industrial Relevance: Predictive tools for rheology are of vital importance to the polymer industry to guide research and development projects.

Center Relevance: This project addresses a commercially relevant problem involving macromolecular topology so it fits well within the intent of the Center.

Plan: Working in collaboration with a team in the UK (Daniel Read at Leeds), we expect to refine open source codes for the linear rheology of branched architectures, such as the "Hierarchical Model" from the Larson group and the "BOB" model from the UK. These codes will be explained to Center Members in hands-on training sessions. Inclusion of new concepts of extensional rheology, including recently discovered "constraint release Rouse" effects on the retraction time will be used to develop predictive methods for extensional rheology.

Milestones and Time to Completion: During the first year, the focus will be on making existing codes for linear rheology widely available and user-friendly. In subsequent years, codes for interpreting extensional rheology will be added.

Annual and Total Cost to Completion: The project will require a graduate student at the University of Michigan. The approximate cost per year will be $55,000 so a total of $165,000.

First Year Deliverables Code for prediction of linear rheology of long-chain branched polymers of arbitrary architecture and instruction manual for use of code.

End of Project Deliverables: Improved code for prediction of linear rheological data, including effects of hyperbranching, and code for extensional rheology prediction for branched polymers.

6) Sol-Gel Chemistry for Photovoltaics

Proposed Team: R. Laine, P. Green, Dow Corning, Sandia National Labs.

Project Objectives: Sol-gel organometallic chemistry is widely used to produce semiconductor layers in certain types of photovoltaic devices such as Grätzel Cells. In these devices a semi-conducting nano-powder is immersed in an electrolyte (iodide solution). When the electrolyte/semi-conductor system contains a dye that can absorb solar radiation and has a band gap similar to that of the semi-conductor, a transfer of electrons from the dye to the semi-conductor is possible. With the semi-conductor in contact with an anode and the electrolyte is in contact with a cathode a photo current can be produced from this simple and extremely inexpensive device. The key structural element in this device is the sol-gel derived inorganic semi-conductor. The proposed work seeks to take advantage of two world-class experts in sol-gel chemistry and physics at the University of Michigan to design improved photovoltaic devices. The project will focus on understanding the effects of manipulation of molecular topology in silicon chemistry to tune the structure and chemistry of the semi-conductor layer in Grätzel Cells for improved performance and lower manufacture costs.

Industrial Relevance: The development of inexpensive solar power is a topic of primary interest to the Department of Energy and Sandia National Labs. Sandia has, in the past, teamed with Dow Corning to develop sol-gel techniques to improve product lines in the elastomer arena. Dow Corning now has strong interest in further developing silicon chemistry in the photovoltaic's industry so that a natural team for this project would link workers at the University of Michigan with DC and Sandia.

Center Relevance: This project addresses a commercially relevant problem involving macromolecular topology since the target is to improve the performance of photovoltaic devices using silicon molecular topology in sol-gel chemistry.

Experimental Plan: The project will involve synthetic work in the lab of Rick Laine as well as characterization work in the lab of Peter Green. The project has strong links to an existing center on photovoltaic's technology headed by Prof. Green. Students will coordinate their work with existing efforts at the center.

Milestones and Time to Completion: The first year of the project will involve development of lab techniques for the production of Grätzel Cells using commercial titania pigment and pigments made in the lab of Laine. In the second year improvement on the photovoltaic technique will be made using in situ produced titiania from organically modified precursors to manipulate the structure and conductivity and compatibility with the organic pigment. The third year will complete the research and be used to prepare and submit publications related to the project. It is expected that patents will result from this project in addition to publications.

Annual and Total Cost to Completion: The project will require a graduate student at the University of Michigan working with Profs. Laine and Green in a collaborative effort depending on the progress a second graduate student may be needed in the second and third years. The approximate cost per year will be $55,000 so a total estimated cost of $165,000.

First Year Deliverables: Development of technology for the production of Grätzel Cells and initial studies of sol gel modification of the process.

End of Project Deliverables: The project will result in at least one publication dealing with the manipulation of sol-gel chemistry to produced improved photovoltaic devices. It is expected that this project will lead to intellectual property.

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 complex macromolecular structures. The center will host a series of short courses aimed at training scientists and engineering in the use of tools developed in the center. Some initial examples of these center sponsored short courses are : "*Structure and Rhoelogy of Molten Polymers*" taught by Ron Larson and Mike Soloman from the University of Michigan; "*Scattering Techniques for Topological Structure of Complex Macromolecules*" taught by Greg Beaucage; "*Simulation Methods for Prediction of Properties in Branched Polymers*" taught by Ron Larson (U. Michigan) and Vikram Kuppa (U. Cincinnati); "*Synthetic Mechanisms for Chain Branching in Polyolefins*" Ron Larson (U. Michigan), Jimmy Mays (U. Tennessee/ORNL).

The Center will also sponsor forums on various aspects of chain topology of interest to the industrial and national lab members. For example a forum on structure/property relationships of polymer gels would be appropriate with invited speakers from outside and inside of the center. Targeted strategy groups will be developed such as a polyethylene group focusing on the characterization and control of long chain branching. These forum meetings, courses and strategy group meetings would take place just before or just after the center meetings.

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 of commercial polymer melts**. We will use rheological instrumentation available at the University of Michigan to provide rheological characterization of commercial polymer melts and solutions, including polymers with long-chain side branching. Each participating company will receive an allocation of measurement time on our rheological equipment, and an option to purchase additional time for a reasonable fee.
2. **Rheological interpretation**. Using advanced modeling methods that account for polydispersity in molecular weight, branch length, and branch placement, we will interpret the measured rheology of polymer solutions and melts, providing information on molecular

structure, batch-to-batch variability, and other features of polymer melts. This interpretation will draw on both rheological data and other characterization data, such as GPC, and TGIC, and light scattering. We will offer both interpretation of data measured at the University of Michigan, and that measured within the companies.

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. We propose to provide training sessions to bring industrial scientists up to date regularly with the latest methods, drawn from our own work, and that of others from around the world. Larson is in regular contact and collaboration with the world's leading polymer rheologists, including involvement in the "Dynacop" program centered in the UK. 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, to provide the maximum impact on their bottom line.

4. **Rheological software**. We will also provide software developed at the University of Michigan for interpreting rheological data, including the hierarchical model, as well as improved versions, as they become available. 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, depending on the priority determined through interactions at the training sessions.

Prior NSF:

Prof. Larson: DMR-0604965 "Testing Advanced Tube Theories for Predicting the Rheology of Model Branched Polymers" $348,000, 9/1/2006 to 8/31/2009

This grant involves collaboration with Jimmy Mays of the University of Tennessee, and his lab to produced a series of nearly monodisperse "H" polymers with controllable branch lengths, to be characterized thoroughly by GPC, temperature gradient interaction chromatography (TGIC) and rheological measurements. These polymers are made using a novel synthetic scheme, one of which is shown in Figure 2b page 6 of this proposal.

The goal of this research is to develop a deep enough understanding of branched polymer dynamics to predict the rheology of arbitrarily branched polymers from knowledge of their branching structure. Since commercial branched polymers contain molecules with multiple branch points, the H polymers are idealized versions of the molecules that are present in commercial polymers. By blending such H polymers with star and linear polymers, we can create very well controlled, but complex mixtures of molecular structures that are analogous to those in commercial polymers. Since we precisely know their composition, these mixtures will allow us to test our ability to predict the rheology of such mixtures, and thereby build a bridge to the prediction of the rheology of commercial melts. So, far, we have successfully predicted the rheology of some of these "H" polymers and their blends with linear and star-shaped polymers, Figure 2a page 6. We have also demonstrated the ability of rheology to detect tiny levels of long-chain branching (as low as 0.35 long-chain branches *per million* backbone carbon atoms) in a series of blends of commercial polyethylenes containing no long branches, with a commercial metallocene long-chain branched polyethylene. The work is continuing under a new NSF grant, DMR-0906587 (09/01/2009 to 8/31/2013).

Prof. Larson: DMR-0906587 "Collaborative Research: Synthesis and Rheology of Strategically Designed Long-Chain Branched Polymers" $400,000, 9/1/2009 to 8/31/2013

Under a sub-contract of this grant, Jimmy Mays and his lab at the University of Tennessee are producing a series of nearly monodisperse, well controlled, H polymers for our rheological studies. This includes the first synthesis of an "asymmetric H" polymer, with arms of differing, but well controlled, molecular weights. Such structures will allow us to test our understanding of branched polymer rheology

and our ability to predict the effect on rheology of heterogeneity in branch length. Commercial samples with long-chain branching, such as metallocene polymers, invariably contain a distribution of branch lengths, and so the ability to predict the effect of such heterogeneity on rheology is an important goal of "analytical rheology" – the inference of molecular weight and branching from rheological properties.

The storage modulus G' of an example "H" polymer is plotted in Figure 2a page 6, along with the predictions of our rheological model for branched polymers, the "hierarchical model." We found that the "hierarchical model" can predict both the rheology of highly purified H polymer and the effect of additional components, such as 12% by volume of a regular star polymer, and 50% of a linear polymer; see, for example, Figure 2a. These and many other results demonstrate that the rheology of mixtures of branched and unbranched polymers can be predicted by advanced "tube" models, such as the "hierarchical model" in many cases. We are now extending this work to much more complex mixtures, leading up to the prediction of the rheology of commercial polymer melts. The prediction of commercial melts combines the "hierarchical model" with "synthesis simulation" in which we use the known reaction catalyst chemistry (such as single-site metallocene chemistry) to predict the distribution of molecular products. An ensemble of molecular structures, representing those most likely present in the product, derived from the synthesis simulation, is then fed into the "hierarchical" rheological model, allowing realistic predictions of the rheological of very complex molecular mixtures, characteristic of commercial melts.

Prof. Beaucage: CBET-0626063 "Spray Jet Flames for Supported Gold Catalysts: New Catalysts by Design." $400,000, 09/01/06 to 08/31/10

The project has supported a US resident PhD student, a minority high school teacher (2 summers) and 4 female and one minority undergraduate student. The graduate student and one of the REU undergraduates spent more than 6 months in Zürich Switzerland as part of this project. A spray flame reactor was developed for the production of supported gold catalysts on metal oxide supports for room temperature oxidation of CO. Nano-scale gold catalysts were produced on titania, silica, alumina and iron oxide supports. The mechanism of formation of these supported catalysts was studied in the flame using in situ anomalous x-ray scattering (ASAXS) at the Advanced Photon Source of Argonne National Laboratory as well as at the NSF funded CAMD synchrotron facility at LSU. The reactivity of the supported catalysts was studied using a quartz reactor coupled with a mass spectrometer for monitoring the exhaust gasses. For comparison, Au/TiO_2 catalyst was also synthesized using deposition precipitation (DP) method. For the CO oxidation reaction, it was observed that the activity of catalyst prepared by deposition precipitation DP method is higher then those prepared by spray flame pyrolysis (SFP) for the same weight loading of gold. SFP has the advantage that it is a continuous process and can produce these supported catalysts at a much higher rate and at a lower cost. While the SFP gold particles are larger and have a broader size distribution, the lower activity of SFP catalysts seems to be primarily associated with the shape of the particles that differ between the two preparation methods. Gold particles from the DP method seem to be two-dimensional with a height of less than two atomic-layers. In contrast, the SFP gold particles are three-dimensional nano-crystals embedded on the TiO_2 surface. There are also differences in the morphology of the titania support phase between pyrolytically formed catalysts and those produced by DP using commercial TiO_2. The effects of catalyst support structure in the DP method were studied using TiO_2 produced in SFP of variable morphology. The activity of catalysts prepared using the flame made TiO_2 is even higher then the catalysts made using commercial TiO_2. The work involved extensive use of EXAFS facilities at ESRF in Grenoble, France. The project has also involved independent projects by REU, RET, IREE students and scientists involving other nanoparticulate aerosols such as carbon soot from diesel engines, iron oxide nanoparticles, carbon-coated titania and platinum catalysts supported on alumina. Two papers are in submission associated with this work and four papers are being prepared. Prior publications associated with the preparation of catalysts by the co-PI (out of 115 peer reviewed papers) include a paper in *Nature Materials* [18] as well as 6 further papers [20-25].

References:

1) *Determination of branch fraction and minimum dimension of mass-fractal aggregates.* Beaucage G, *Phys. Rev. E*. **70** 031401 (2004).
2) *Dimensional Description of Cyclic Polymers.* Kulkarni AS, Beaucage G *Macromolecules* **43** 532–537 (2010).
3) *Persistence Length of Short-Chain Branched Polyethylene.* Ramachandran R, Beaucage G, Kulkarni AS, McFaddin D, Merrick-Mack J, Galiatsatos V *Macromolecules* **41** 9802-9806 (2008).
4) *Branch content of metallocene polyethylene.* Ramachandran R, Beaucage G, Kulkarni AS, McFaddin D, Merrick-Mack J, Galiatsatos V *Macromolecules* **42** 4746-4750 (2009).
5) *Dimensional Description of Cyclic Polymers.* Kulkarni AS, Beaucage G *Macromolecules* **43** 532–537 (2010).
6) *Toward resolution of ambiguity for the unfolded state. Beaucage G Biophys. J.* **95** 503-509 (2008).
7) *Investigating the molecular architecture of hyperbranched polymers using small angle neutron scattering.* Kulkarni AS, Beaucage G *Macromolecular Rapid Comm.* **28** 1312-1316 (2007).
8) *Branch length distribution in TREF fractionated polyethylene* . Ramachandran R, Beaucage G, McFaddin D, Merrick-Mack J, Galiatsatos V accepted *Polymer* (2011).
9) *Scaling model for symmetric star polymers*, Rai DK, Ramachandran R, Beaucage G submitted *J. Appl. Cryst.* (2011).
10) *In situ studies of nano-particle growth dynamics in premixed flames.* Kammler HK, Beaucage G, Kohls DJ, Agashe N. Ilavsky J., *J Appl. Phys.* **97** 054309 (2005).
11) *Particle size distributions from small-angle scattering using global scattering functions.* Beaucage G, Kammler HK, Pratsinis SE, *J. Appl. Cryst.* **37** 523-535 (2004).
12) *3D Hierarchical orientation in polymer-clay nanocomposite films.* Bafna A, Beaucage G, Mirabella F *Polymer* **44** 1103-1115 (2003).
13) *A structural model for equilibrium swollen networks.* Sukumaran SK, Beaucage G *Europhys. Lett.* **59** 714–720 (2002).
14) *Neutron scattering from equilibrium-swollen networks.* Sukumaran SK, Beaucage G., Mark JE, Viers, B. *Eur. Phys. J. E* **18** 29–36 (2005).
15) *Quantification of hyperbranched (branch-on-branch) content in model polyolefins.* Ramachandran R, Beaucage G, Lohse D in preparation (2011).
16) *Structure and rheology of molten polymers : from structure to flow behavior and back again* , Ronald G. Larson, John M. Dealy, Munich : Hanser Publishers ; Cincinnati : Hanser Gardner Publications, (2006).
17) *The structure and rheology of complex fluids* Ronald G. Larson, New York : Oxford University Press (1999).
18) *Neutron scattering from superabsorbent gels of polyacrylic acid*. Beaucage G, Dirama T, Wireko F, Weaver M, in preparation (2011).
19) *Probing the dynamics of nanoparticle growth in a flame using synchrotron radiation.* Beaucage G, Kammler HK, Mueller R, Strobel R, Agashe N, Pratsinis SE, and Narayanan T *Nature Mater.* **3** 370-373 (2004).
20) *In situ studies of nano-particle growth dynamics in premixed flames.* Kammler HK, Beaucage G, Kohls DJ, Agashe N. Ilavsky J. *J Appl. Phys.* **97** 054309 (2005).

21) *Determination of branch fraction and minimum dimension of mass-fractal aggregates.* Beaucage G *Phys. Rev. E* **70** 031401 (2004).
22) *Non-agglomerated dry silica nanoparticles.* Mueller R, Kammler HK, Pratsinis SE, Vital A, Beaucage G, Burtscher P *Powd. Tech.* **140** 40-48 (2004).
23) *Structure of flame-made silica nanoparticles by ultra-small angle X-ray scattering.* Kammler HK, Beaucage G, Mueller R, Pratsinis SE *Langmuir* **20** 1915-1921 (2004).
24) *The effect of external electric fields during flame synthesis of titania.* Kammler HK, Jossen R, Morrison PW, Pratsinis SE, Beaucage G *Powd. Tech.* **135** 310-320 (2003).
25) *Fractal analysis of flame-synthesized nanostructured silica and titania powders using small-angle X-ray scattering.* Hyeon-Lee J, Beaucage G, Pratsinis SE *Langmuir* **14** 5751-5756 (1998).

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1980 University of Rhode Island, Kingston, RI 02881 ***B.S. Zoology***; Highest Distinction. (National Merit Scholar Finalist, Elected to Phi Beta Kappa)

1982 University of Rhode Island, Kingston, RI 02881 ***B.S. Chemical Engineering;*** High Distinction. (Elected to 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***, Organic Materials Group *Characterization of nanomaterials using scattering & scattering theory.*

Appointments

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

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*** 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.

Other Experience and Professional Memberships

2008 Fellow American Physical Society

2000-2008 Advisory Board Intense Pulse Neutron Source, Argonne Natonal Laboraotry.

2003-present Founding Member of LENS Neutron Scattering Facility at Indiana University

2000-present Founding Member of LSU Synchrotron CAMD SAXS User Group

1980-present Member American Institute of Chemical Engineers

1990-present Member American Physical Society

1992-present Member American Crystallographic Society

2004-2005 Chair of the Small Angle Scattering Special Interest Group ACryS.

2003-2004 Program Chair Small Angle Scattering Special Interest Group ACryS

1995-present Panel and Individual Referee for NSF/PRF/DOE/Commerce Proposals.

10 Related Publications (from 113 peer reviewed H-Index 26)

1) *Towards resolution of ambiguity for the unfolded state.* Beaucage G *Biophysical J.* **95** 503-509 (2008).
2) *Probing the dynamics of nanoparticle growth in a flame using synchrotron radiation.* Beaucage G, Kammler HK, Mueller R, Strobel R, Agashe N, Pratsinis SE and Narayanan T, *Nature Mater.* **3,** 370-373 (2004).
3) *In situ studies of nano-particle growth dynamics in premixed flames.* Kammler HK, Beaucage G, Kohls DJ, Agashe N. Ilavsky J., *J Appl. Phys.* **97**(5) 2005 (Article 054309).
4) *3D Hierarchical orientation in polymer-clay nanocomposite films.* Bafna A, Beaucage G, Mirabella F *Polymer* **44**, 1103-1115 (2003).
5) *A structural model for equilibrium swollen networks.* Sukumaran SK, Beaucage G *Europhysics Letters* **59** 714-720 (2002).
6) *Approximations leading to a unified exponential/power-law approach to small-angle scattering.* Beaucage G, *J. Appl. Crystallogr.* **28**, 717-728 (1995).
7) *Small-Angle Scattering from Polymeric Mass Fractals of Arbitrary Mass-Fractal Dimension.* Beaucage G, *J. Appl. Crystallogr.* **29**, 134-146 (1996).
8) *Determination of branch fraction and minimum dimension of mass-fractal aggregates.* Beaucage G, *Phys. Rev. E*, **70**, 031401 (2004).
9) *Quantification of branching in disordered materials.* Kulkarni A, Beaucage G *J. Polym. Sci. Polym. Phys.* **44** 1395-1405 (2006).
10) *Persistence Length of Short-Chain Branched Polyethylene* Ramachandran R, Beaucage G, Kulkarni AS, McFaddin D, Merrick-Mack J, Galiatsatos V *Macromolecules* In Press (11/2008).

Synergistic Activities

1) *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.
2) *Creation*: Developed aero-sol-gel reactor for room temperature aerosol synthesis.
3) *Transfer of Knowledge*: Chairman of small-angle scattering group American Crystallographic Association, Organizer for annual meeting of ACA.
4) *Transfer of Knowledge*: 20 Sessions Organized for AIChE, ACA, MRS, APS meetings.
5) *Transfer of Knowledge*: 12 web courses (9 pertaining to polymers) extensive notes, lab experiments and data. 255,000 different IP#'s have hit this course suite since 2000 (averaging >70 IP hits/day).

Collaborators & Other Affiliations (past 48 months)

Dr. J. Ilavsky, UNICAT, APS, Argonne National Laboratories, Argonne Illinois.
Dr. T. Narayanan, ESRF ID02, Grenoble France.
Dr. S. E. Pratsinis, Process Engineering, ETHZ, Zurich.
Prof. Ronald Larson, U. Michigan, Ann Arbor.
Dr. S. K. Sukumaran, Assistant Professor, Yamamoto University Japan.
Dr. T. Trevoort, Materials Science, ETHZ, Zurich.
Vassilios Galiatsatos, Senior Scientist, LyodellBasell Cincinnati OH
David Britton, Professor Physics, University of Cape Town, South Africa

Graduate & Postdoctoral Advisors

Dr. Richard S. Stein, Emeritus Professor of Polymer Science and Engineering, University of Massachusetts, Amherst, MA. Member NAS and NAE.

Dr. D. W. Schaefer, Professor of Engineering (Formerly Dean of Engineering), U. Cincinnati.

Dr. J. G. Curro, Former Head of Polymer Group, Sandia National Laboratory, Albuquerque NM.

Thesis Advisor and Postgraduate-Scholar Sponsor (PhD: 7 , MS: 8, Post Doc: 2)

Current Students: (4 Graduate Students, 2 Funded REU Undergraduate, 1 funded RET High School Teacher, 2 Unfunded Undergraduates)

Durgesh Rai: PhD studies scattering theory.

Sachit Chopras: PhD studies flame-made nanoparticles for nano-catalysts and other applications. Funded by NSF CTS.

Ramnath Ramachandran: PhD studies branching and persistence effects on rheology in polyolefins. Funded by LyondellBasell.

Ryan Breese (MS 2004; PhD 2009): PhD studies on oriented polymer film structure/property relationships. Funded by Equistar and now by Eclipse Film Technologies.

Mangesh Champhekar: (MS 11/2008) Studies of ultra oriented polyolefin/clay nano-composites.

Hao Liu, Senior Project: In situ SAXS studies of Diesel Exhaust at the CHESS Synchrotron.

Kurt Woodford, *Senior Project: Orientation in Polyolefin Films*.

Undergraduate Research Assistant (NSF REU Students): Stephanie Berger, Carbon coated silica for solar cell applications. **Robin Holland,** (Minority REU Student) In situ studies of diesel exhaust nanoparticulates using synchrotrons. **Maesa Idries**, Current REU student.

High School Teacher (NSF RET Participant): Edwin Segbefia Princeton High School Physics Department (Minority teacher). Flame-made hematite nano-particles for arsenic remediation in drinking water.

Select Past Graduated Students/Post Doc

Amit Kulkarni (MS 2004; PhD 2007): Funded by P&G, Intel, Equistar. Currently Research Engineer *GE Plastics Evansville IN (10/2007).*

Doug Kohls, (MS 2002; PhD 2006): Currently Assistant Professor Dept. Materials Science and Engineering University of Cincinnati.

Hashard Chavan (MS 2006) *Bioplastics San Jose CA.*

Ayush Bafna (PhD 2004, MS 2002) *Research Engineer, Dow Chemical Central Research Freeport TX.*

Nikhil Agashe (PhD 2004, MS 2001) *Research Engineer GE Plastics, Evanston IN.*

Suresh Murugesan (PhD Chemistry 2003) *Scientist Texas Research Institute.*

S. Sukumaran (PhD 2002) *Asst. Prof. Polymer Science Yamata University, Japan.*

G. Skillas (Post-Doc from ETH Zurich 2001) *Research scientist, GMX Degussa, Hanau Germany.*

J. Hyeon-Lee (PhD 1998) *Research Scientist, Samsung Research Institute, Seoul, South Korea.*

Ling Guo (MS 1997) *P&G Miami Valley Laboratories (Central Research Division).*

S. Rane (PhD 1999) *Senior Research Engineer, Procter& Gamble Beckett Ridge Technical Center Cincinnati.*

RONALD GARY LARSON

BIOGRAPHICAL SKETCH

Depts. of Chemical Engineering, Mechanical Engineering, Biomedical Engineering, and Macromolecular Science and Engineering, Univ. of Michigan
Ann Arbor, MI 48109-2136, rlarson@engin.umich.edu

a) Professional Preparation

June, 1975 - B.S., Chemical Engineering, University of Minnesota
June, 1977 - M.S., Chemical Engineering, Univ. of Minnesota, June 1977
August, 1980 -Ph.D., Chemical Engineering, University of Minnesota, under Drs. L.E. Scriven and H.T. Davis.

b) Appointments

Oct.,1996-present - Professor, Univ. of Mich.
Dec.,1980-Oct., 1996 – Distinguished Member of Staff at Bell Laboratories.
Sept.,1976- June,1977 - Consultant to Gary Operating Co., Englewood, CO
June-Sept., 1975 - Shell Development in Houston, under Dr. G. Hirasaki.

c-i) Most Relevant Publications

1.) X. Chen, F.J. Stadler, H. Munstedt, and R.G. Larson, *J. Rheol*. 54:393-406 **2010** "Method for Obtaining Tube Model Parameters for Commercial Ethene/Alpha-Olefin Copolymers."
2.) Z.W. Wang, X. Chen, and R.G. Larson, *J. Rheol*. 54:223-260 **2010** "Comparing Tube Models for Predicting the Linear Rheology of Branched Polymer Melts."
3.) X. Chen, C. Costeux, and R.G. Larson *J. Rheol*., 54:1185-1205 **2010** "Characterization and Prediction of Long-Chain Branching in Commercial Polyethylenes by a Combination of Rheology and Modeling Methods."
4.) R.G. Larson, J. Polym Sci. B. Polym. Phys. Ed. 45:3240-3248 **2007,** "Looking inside the entanglement "Tube" using molecular dynamics simulations."
5.) Z.W. Wang and R.G. Larson Macromolecules 41:4945-4960 **2008** "Constraint Release in Entangled Binary Blends of Linear Polymers: A Molecular Dynamics Study."

c-ii) Other Significant Publications

1.) B. Shang, Z. Wang, and R.G. Larson, J. Phys. Chem., 112:2888-2900, **2008** "Molecular Dynamics Simulation of Interactions between a Sodium Dodecyl Sulfate Micelle and a Poly(ethylene oxide) Polymer."
2.) N. Hoda and R.G. Larson, Macromolecules, 113:4232-4241 **2009** "Explicit- and Implicit-Solvent molecular dynamics simulations of complex formation between polycations and polyanions."
3.) N. Hoda and R.G. Larson *J. Rheol*. 54:1061-1081 **2010** "Brownian Dynamics Simulations of Single Polymer Chains With and Without Self-Entanglements."

4.) S.L. Duncan and R.G. Larson *Biochim. Biophys. Acta – Biomembranes* 1798:1632-1650 **2010**, "Folding of Lipid Monolayers Containing Lung Surfactant Proteins SP-B1-25 and SP-C Studied Via Coarse-Grained Molecular Dynamics Simulations.
5.) J.H. Kim and R.G. Larson, Nucleic Acids Res., 35:3848-3858 **2007** "Single-molecule analysis of 1D diffusion and transcription elongation of T7 RNA polymerase along individual stretched DNA molecules."

d) Synergistic Activities

1) Publication of a textbook on Polymer Melts, co-authored by John Dealy.
2) Publication of a textbook on Complex Fluids by Oxford University Press, used in the complex fluids course, both at Michigan and other universities
3) Development of a short course on rheology and complex fluids, taught in Thailand, China, and a short course on rheology at the University of Massachusetts
4) Chair of the Polymer Division of the American Physical Society.
5) Divisional Editor (DAE) for Physical Review Letters

e-i) Collaborators within the Past 48 Months
From University of Michigan: Michael Solomon , Mark A. Burns, David Burke, A. Oveta Fuller, Sharon Glotzer, James R. Baker, Jr., Friedhelm Hildebrandt, Ayyalusamy Ramamoorthy, Stella Pang, Nicholas Kotov, Jay Guo, Nils Walter
From Elsewhere: Francesco Stellacci (MIT), Jimmy Mays (Univ. of Tennessee), Siewert-Jan Marrink (Univ. of Groningen), D. Peter Tieleman (Univ. of Calgary), John Dealy (McGill Univ.), W. van Saarloos (Univ. of Leiden), Masao Doi (Univ. of Tokyo), Cataleeya Pattamaprom (Thomasad University, Bangkok), Anuvat Sirivat (Chulalongkorn University, Bangkok), Michael Cates (Univ. of Edinburgh), Joseph Brader (Univ. Konstanz), Thomas Voigtmann (Univ. Konstanz), Matthias Fuchs (Univ. Konstanz), Radhakrishna Sureshkumar (Univ. of Syracuse), Richard Graham (Univ. of Reading).

e-ii) Graduate Advisors (no post-doc advisors)
L.E. Scriven and H.T. Davis, Univ. of Minn.

e-iii) Ph.D. and post-doc advisees graduated within the last 5 years:
Sachin Shanbhag (Florida State University), Chih-Chen Hsieh (Taiwan National Univ.), Anshuman Roy (Univ. of Calif., Santa Barbara), Senthil Kandasamy (D.E. Shaw), Lin Fang (DuPont, China), Hwan-kyu Lee (Nanyang Technological University, Singapore), Weixian Shi (Bristol-Myers-Squibb), Ji Hoon Kim (Boston Consulting Group), Bruce Schiamberg (Lux Research), Youngsuk Heo (Abbott Labs), Tyson Poeckh (City of Lacey, Washington), Qiang Zhou (Standard & Poors), Sean Holleran (Univ. of Penn), Semant Jain (Praxair), Zuowei Wang (University of Reading, UK), Zhicheng Long (Univ. of Minnesota), Laura Shereda (not yet employed)

e-iv) Current Ph.D. and post-doc advisees
Susan Duncan, Zue Chen, Nobuhiko Watari, Indrasil Sala Dalal, Xueming Tang, Shi Yu, Priyanka Desai, Shihu Wang,

Facilities, Other Resources and Equipment

Facilities:

Beaucage/University of Cincinnati:

410 Rhodes Hall Laboratory is a 600 square foot research laboratory primarily focusing on scattering and polymer characterization instruments.

551 Engineering Research Center Laboratory is a 300 square foot research laboratory with a hood, suitable for chemical synthesis. A light scattering camera is also housed in this lab as well as two polymer processing machines and a polymer film gas permeability tester.

Office: Beaucage's office is located in 492 Rhodes Hall with student desks in the labs.

Breese/Eclipse Film Technology:

25,000 ft^2 polymer processing facility located 10 miles from the UC campus with office and lab space for polymer characterization.

Equipment:

Beaucage/University of Cincinnati:

Polymer Processing Equipment:

Collin Teach Machine Direction Orientation Unit On loan from Eclipse Film Technolog and Collin GmbH (http://www.drcollin.de/en/index_en.html). Lab scale polymer film stretching machine.

Brabender 50 gm Extruder Located in ERC 551 Lab. Film blowing attachment and home made take-up tower as well as mixing head. Home made fiber spinning apparatus. (See http://www.eng.uc.edu/~gbeaucag/Classes/Processing.html for pictures and video of this equipment. Equipment was donated by Dow Chemical and P&G to Beaucage, is very old but functional.

Departmental Carver Hot Press. Located in Polymer Processing Laboratory.

TM Long Stretch Polymer Film Biaxial Stretcher from Inventure Labs www.inventurelabs.com. Donated from P&G Polymer Processing Center Beckett Ridge Laboratories to Beaucage. Instrument is for static and dynamic precision biaxial deformation of polymer films. This instrument will be used to study post blowing/casting nano-composite orientation located in 410 Rhodes Hall.

Departmental Battenfeld injection molding machine. Fairly old but functional machine purchased second hand about 10 years ago for $7,000. Located in Polymer Processing Laboratory at the University of Cincinnati.

Scattering Equipment

12 kW Rigaku rotating anode X-ray source with three small angle X-ray scattering cameras located in 410 Rhodes Hall laboratory of Beaucage with:

A pinhole camera with a 2-D detector focusing optics automatic sample changer. Instrument has been widely used in published SAXS studies. 0.5 to 50 nm size resolution, absolute intensity capability.

Kratky SAXS camera, capable of wider q-range compared to pinhole camera. Data is slit smeared requiring desmearing making results less reliable. 0.1 to 100 nm resolution.

Bonse-Hart USAXS camera. 1 nm to 1 micron resolution.

Two static light scattering cameras and optical components.

Pinhole small-angle light scattering camera with 2D CCD camera located in 410 Rhodes Hall laboratory of Beaucage. Camera is enclosed in a dark box with vertical alignment, 20 mW HeNe laser, adjustable attenuator, polarizers pinhole optics, hot stage capabilities, scattering is projected on a screen and imaged with a Princeton Instruments 2D CCD detector. 0.6 to 100 micron resolution.

Ultra-small angle light scattering camera located in 551 Engineering Research Center laboratory of Beaucage. 30 mW HeNe laser, step scan goniometer with fiber optics connection to PMT and computer. Unique optics for USALS measurements, 1 micron to 1 cm resolution.

Assorted optics, optical tracks, 5 mW HeNe laser, stepper motors and motor controller.

Dynamic light scattering instrument, ALV-500/E/EP sold by Malvern Instruments in the US which can be used for solution DLS for colloidal suspensions of nanoparticles yielding the hydrodynamic radius from the diffusion coefficient. Also a Malvern RH2000 Bench top torque rheometer is available. Both instruments are on loan from Malvern but are intended to be used in courses and for research as well as for demonstrations to customers for Malvern in a special arrangement.

Other Equipment:

Dupont Instruments 912 Differential Scanning Calorimeter in the 410 Rhodes Lab.

Polymer Melt Rheometer: Rheometerics Dynamic Analyzer RDA II in the 410 Rhodes Lab.

TA Instruments Dynamic Mechanical Analyzer DMA 983 in the 410 Rhodes Lab.

Mocon Oxytran 2/20 O_2 Permeability Tester for films and membranes in the 551 ERC Laboratory.

Dynamic IR instrument, which couples a dynamic mechanical analyzer with IR birefringence measurements thorough a series of lock-in amplifiers for polymer dynamic studies located in 410B Rhodes Hall laboratory of Beaucage. The instrument has a high resolution dispersive IR spectrometer. Other IR facilities are available in Departmental Facilities and in the Chemistry Department.

4 Pyrolytic reactors with 6 mass flow controllers, assorted tubing, heat tape, neutralizers, filter banks and exhaust pump located in the 551 Engineering Research Center Laboratory of Beaucage.

The Advanced Materials Characterization Center (AMCC) operated by the Department of Chemical and Materials Engineering at University of Cincinnati Located on the 3'rd floor of the Engineering Research Center has a CM-20 TEM, with a LaB_6 source, theoretical resolution of 1.4 Å and EDS capabilities. The operating costs are $85 per hour.

The SEM setup at the University of Cincinnati AMCC facility include a Hitachi S 4000 conventional FEG SEM with a theoretical resolution of 15 Å, and EDS capabilities and

an environmental FEI XL 30 ESEM-FEG with a theoretical resolution of 15 Å and operating pressure of 20 torr. The operating costs for SEM are $80 per hour.

X-ray powder diffraction is also available at the AMCC with a user fee or $40/h.

- **Other Resources**:

Beaucage is a long-term collaborator and consultant with the Equistar division of LyondellBasell Corporation, the number 2 producer of polymers in the US and number 1 producer of polyolefins. Equistar's polymer processing research facility frequently collaborates with Beaucage and this collaboration is expected to continue through this project.

Beaucage is also a long term collaborator and consultant with Procter & Gamble Corporation which has polymer processing facilities in two main locations in Cincinnati.

Beaucage is PI on a long term user agreement with ESRF for in situ SAXS studies using beam line ID02. The work is in collaboration with T. Narayanan of ESRF and with S. E. Pratsinis of ETHZ. The agreement guarantees access to the synchrotron facilities for several weeks per year and is renewable after 3 years. The user agreement currently has 1 year remaining.

Beaucage also has a working arrangement with two beam lines at the Advanced Photon Source in Chicago at the UNICAT and at the DNDCAT user facilities.

SAXS measurements are frequently performed at CHESS (Cornell University) and at SSRL (Stanford University). Beaucage is also a founding member of the user group for the LSU SAXS facility funded by NSF (CAMD).

FACILITIES, EQUIPMENT & OTHER RESOURCES

Major Equipment in Larson Lab and accessible to Larson group

Microscopy Two Nikon inverted TE 200 microscopes are available with fluorescence imaging using a Hamamatsu SIT video camera and a Roper Coolsnap video camera. One of the microscopes is equipped with a Ludl Biopoint XY focus drive and control, Prior High Precision 4 X 3" X-Y Motorized Stage including video auto focus, controller, and joystick. PCI full-image software allows image capture and Corona Imaging Hardware allows real-time image capture and transfer to memory system. The software resides on an Intel Pentium II 300 MHz PCI Tower Computer. The department also has a confocal microscopy facility, with a Leica TCS SP2 confocal microscope.

Cell Culture The department has a cell culture facility, with incubators, shakers, and other equipment suitable for culturing E. coli bacteria.

Rheometry The Larson group shares with the Solomon group a Rheometrics ARES rheometer for dynamic oscillatory and steady shear measurements of polymeric and colloidal fluids.

Computer Clusters: The Larson group possesses a 16-processor Apple G5 cluster, housed in the University of Michigan Center for Advanced Computing (CAC). The Larson group is acquiring a cluster of 8 GPU nodes, and Intel CPU's, each with 8 cores (supplier TBD).

General Laboratory: The Larson research laboratory is located in the H.H. Dow Building of the College of Engineering, University of Michigan, room 3125. The total lab space is approximately 1200 square feet and has two chemical fume hoods, and adequate storage, bench, and desk space for 6 people. The following basic chemistry and molecular biology items available in the lab: balance, chemical reagents, glassware, micropipettors, incubators, 12 sq.ft. refrigerator-freezer, and various other small equipment.

Office
The Larson group has two student offices, with around 900 sq ft of total space, as well as Larson's research office, with 150 sq ft. Both are adequate and equipped with computers and printers. Secretaries are nearby to help with routine office tasks.

Data Management Plan.

The planning grant will not result in the generation of experimental data. The planning meeting will produce ratings of proposed research projects through the LIFE (level of interest, feedback & evaluation) evaluation forms and web based survey forms. Data from these forms will be complied, summarized and reported on the Center web page. Data management will be the responsibility of Prof. Beaucage, the Center Director. The Center Evaluator will monitor compliance with this plan.

Other data concerning suggestions for organization of the Center, membership levels and types, short course and forum topics and general comments concerning the operation of the Center will be compiled and disseminated through the Center web page.

Data Management Plan

Planning Grant: I/UCRC for the Center for Macromolecular Topology

This planning grant will organize a meeting of interested industrial representatives but will generate no experimental or computational data. There is no data sharing required.

Post Doc Mentoring Activities

The planning grant will not involve post-docs but the Center will, in some cases, involve post-doctoral scientists in the research activities. A standard mentoring plan will be used as outlined below.

This Postdoctoral Researcher Mentoring Plan has been prepared by the University of Cincinnati and the University of Michigan. The Plan establishes guidelines for work to be performed by a Postdoctoral Researcher in support of the NSF Project Awarded to Profs. Beaucage and Larson, entitled "The Center for Macromolecular Topology" The Postdoctoral Researchers assigned to the project will work in the University of Cincinnati or the University of Michigan or affailate laboratories and will conduct research on Macromolecular Topology.

1. Orientation will include in-depth conversations between Profs. Larson and Beaucage and the Postdoctoral Researchers. Mutual expectations will be discussed and agreed upon in advance. Orientation topics will include (a) the amount of independence the Postdoctoral Researcher requires, (b) interaction with coworkers, (c) productivity including the importance of scientific publications, (d) work habits and laboratory safety, and (e) documentation of research methodologies and experimental details so that the work can be continued by other researchers in the future.

2. Career Counseling will be directed at providing the Postdoctoral Researcher with the skills, knowledge, and experience needed to excel in his/her chosen career path. In addition to guidance provided by the advising professor, the Postdoctoral Researcher will be encouraged to discuss career options with researchers and managers at the Universities and with former students and colleagues of the advising professor.

3. Experience with Preparation of Grant Proposals will be gained by direct involvement of the Postdoctoral Researcher in proposals prepared by the advising professor. The Postdoctoral Researcher will have an opportunity to learn best practices in proposal preparation including identification of key research questions, definition of objectives, description of approach and rationale, and construction of a work plan, timeline, and budget.

4. Publications and Presentations are expected to result form the work supported by the grant. These will be prepared under the direction of the advising professor and in collaboration with researchers at the universities as appropriate. The Postdoctoral Researcher will receive guidance and training in the preparation of manuscripts for scientific journals and presentations at conferences.

5. Teaching and Mentoring Skills will be developed in the context of regular meetings within the research group during which graduate students and postdoctoral researchers describe their work to colleagues within the group and assist each other with solutions to challenging research problems, often resulting in cross fertilization of ideas.

6. Instruction in Professional Practices will be provided on a regular basis in the context of the research work and will include fundamentals of the scientific method, laboratory safety, and

other standards of professional practice. In addition, the Postdoctoral Researcher will be encouraged to affiliate with one or more professional societies in his/her chosen field.

7. Technology Transfer activities will include regular contact with researchers at the company involved in the research project. The Postdoctoral Researcher will be given an opportunity to become familiar with the university-industry relationship including applicable confidentiality requirements and preparation of invention disclosure applications.

8. Success of the Mentoring Plan will be assessed by monitoring the personal progress of the Postdoctoral Researcher through a tracking of the Postdoctoral Researcher's progress toward his/her career goals after finishing the postdoctoral program.

Supplemental Documents

Center for Macromolecular Topology
Proposed Center Marketing Plan

Target Industries: The target industries for the CMT are: 1) the polyolefins industry and other polymer companies interested in the manipulation and control of chain architecture; 2) the elastomer and rubber industries interested in the relationship between network topology and mechanical properties; 3) Consumer products industry, manufactures and users of gels and branched polymers; 4) Groups concerned with specialty applications of macromolecular topology in a variety of situations of use both commercially and for military applications; 5) Groups interested in the advancement of certain analytic techniques such as ORNL; 6) Industries/Labs involved with hyperbranched and dendrimer macromolecules such as Michigan Molecular Institute and DSM's Hybrane Division; 7) Adhesives industry where network formation is of primary importance; 8) Coatings industry for functionalized macromolecular composition.

Marketing Plan: The marketing plan will be fully developed at the Planning Meeting. Currently the Center is being marketed through personnel contacts of the two 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 2011 ACS Polyolefins meeting in Santa Rosa, California. The Center will offer short courses and forums that will draw in 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 two Center Directors and especially the lead Director at Cincinnati. Researchers interested in participating in the Center 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 Director and Co-Director's research interests that will form the core of the Center Site sponsorships required by NSF. The Center will also initially have several projects that do not involve the Center Directors that expand the Center in new areas within the context of Macromolecular Topology. Two examples of these are given in the Project Description section.

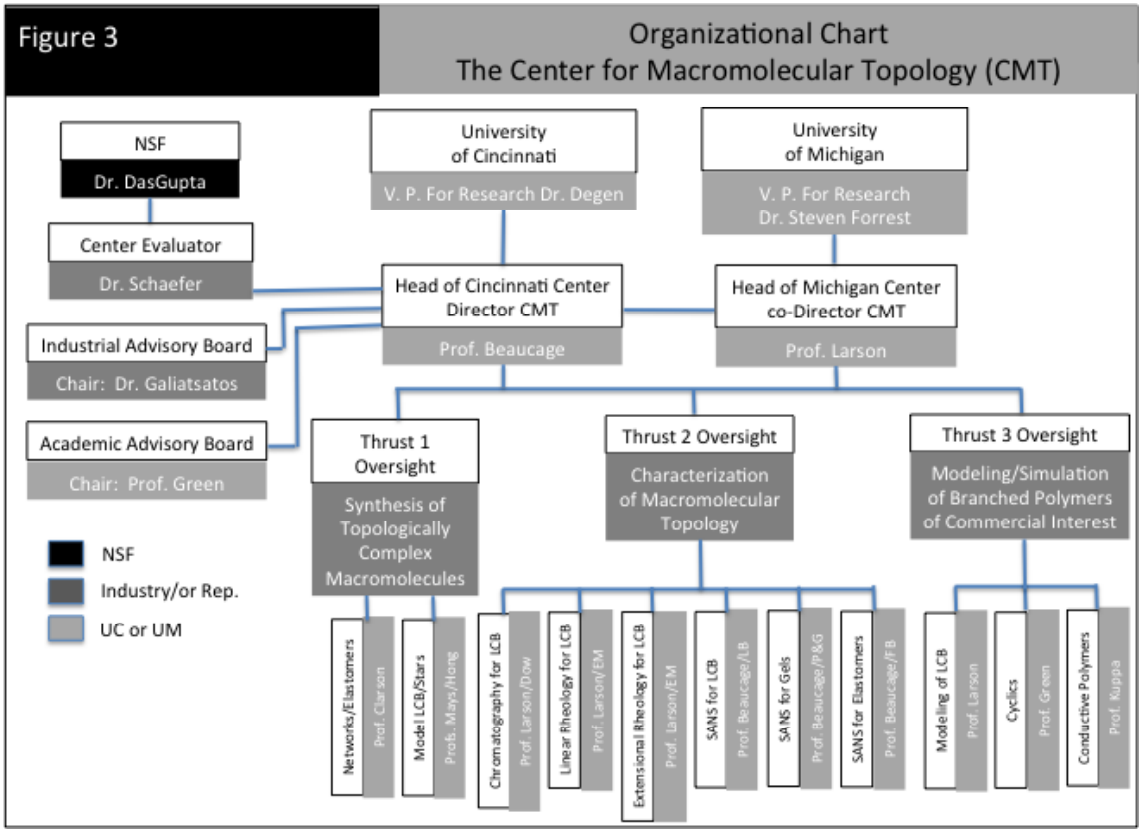
Center Growth: It is expected that the Center will add two companies per year as full members in the first five years with an attrition rate of one company per 3 years (at the end of a typical project). If the Center begins with 8 full members the Center could grow to 15 or 16 members after 5 years supporting 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 $5,000 that would allow attendance at Center meetings, Forums and Short Courses. To buy into a research project a Full Membership would be required that would cost a minimum of $55,000 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 and the Center would also sponsor proposals to the National Labs to support research efforts affiliated with the Center such as to the BES program for DOE. 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 and in kind contributions to the Center effort.

Staffing Plan for the Center for Macromolecular Topology

Figure 3 from the Project Description (reproduced below) shows the proposed Organization Chart for the Center for Macromolecular Topology (CMT).



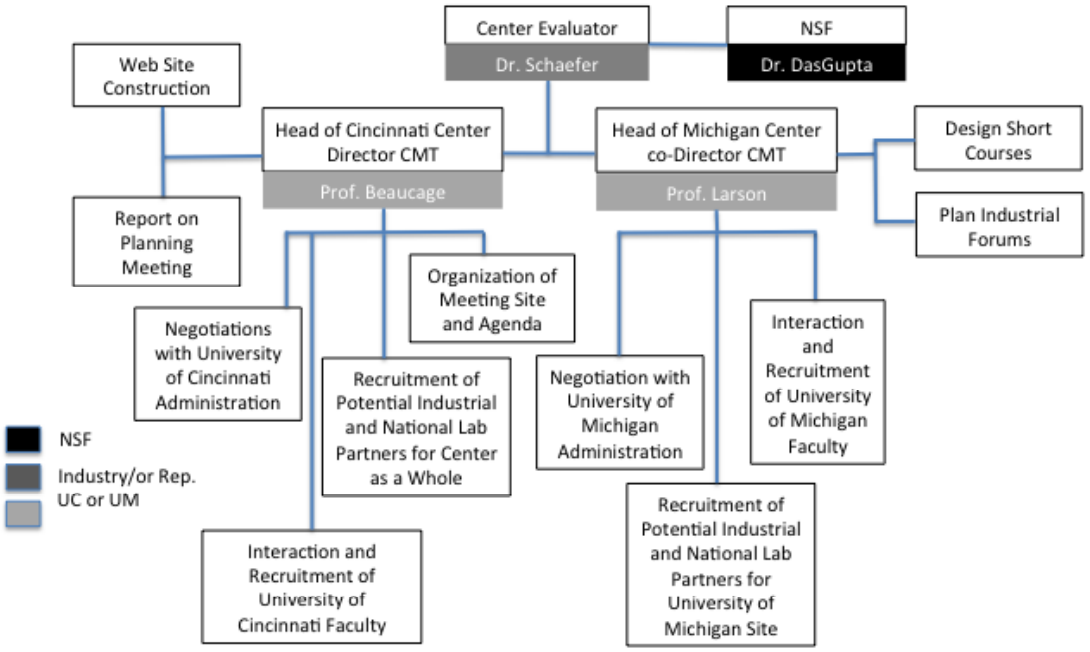
The Center for Macromolecular Topology will have two sites, at the University of Cincinnati and at the University of Michigan. The Center Director and co-Director will report to their respective Vice Presidents for Research concerning issues of importance to the University such as overhead return and 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. Peter Green at Michigan who is Head of the Department of Materials Science and Engineering. Dr. Vassilios Galiatsatos will Chair the Industrial Advisory Board. Galiatsatos 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 synthesis, characterization and modeling/simulation. Activities in all three of these thrusts will exist at both campuses. Some effort will be made to develop projects that have components on both campuses. Each research thrust will have an Oversight Committee composed mostly of industrial/national lab scientists and engineers associated with projects in the Thrusts. 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. A possible candidate for the Evaluator role is Prof. Dale Schaefer at the University of Cincinnati. Prof. Schaefer is a former Dean of Engineering at the University of Cincinnati and formerly a high level manager at Sandia National Laboratory.

Responsibility Martix for the planning study: Figure A, below, shows the responsibility matrix for the planning study. Profs. Beaucage and Larson 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 other faculty to participate in the center. Beaucage will coordinate recruitment of industrial and national lab partners for the Center. Prof. Larson will interact with the University of Michigan administration and faculty and will recruit industrial and national lab partners for the Michigan site. Larson will also take primary responsibility for the design of short courses and industrial forums within the center. Prof. Beaucage will construct a Center web page and 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.

Figure A

Responsibility Matrix for Planning Study
The Center for Macromolecular Topology (CMT)



Draft Membership Agreement for Industrial Partners
for the Center for Macromolecular Topology

This Agreement is made.....this day of ..... by and between the University of Cincinnati/Michigan (hereinafter called "University") and … (hereinafter called "Company") for the Center comprising and acting through the Center for Macromolecular Topology, which is defined as all Macromolecular Topology 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 Macromolecular Topology (hereinafter called "CENTER") at the UNIVERSITY to maintain a mechanism whereby the UNIVERSITY environment can be used to perform research to advance our understanding of complex macromolecules. 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 $55,000 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 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 Macromolecular Topology (CMT)

This Agreement ("Dissemination Agreement") is made this _____ day of _____, 2011 by and between the University of Cincinnati/University of Michigan (hereinafter "University") acting on behalf of the Center for Macromolecular Topology and the undersigned Center for Macromolecular Topology Member ("Member").

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

WHEREAS, the undersigned Center for Macromolecular Topology Member entered into the Membership Agreement effective as of _____; and

WHEREAS Center for Macromolecular Topology 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 Macromolecular Topology Center project, to be delivered prior to each periodic meeting with Members of Center for Macromolecular Topology 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 Macromolecular Topology 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 Macromolecular Topology
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 and Prof. Ron Larson Sandra Degen, Vice President of Research, University of Cincinnati Neville G. Pinto, Vice Provost and Dean of the Graduate School, Univ. Cincinnati Representatives from the University of Michigan
8:35 - 9:15 am	Vision and Capabilities of the Center (Prof. Greg Beaucage and Prof. Ron Larson)
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 (University of Cincinnati)** 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 (University of Michigan)** 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 (Prof. Ron Larson and Greg Beaucage)
6:00 pm	Technical Forum and Social: Poster Session Posters of proposed projects, we expect ~10 from each University.

x

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 (Prof. Ron Larson and Prof. Greg Beaucage)

ADJOURN

List of Letters of Interest
Center for Macromolecular Topology (CMT)

Potential Members: The potential members of the Center's two sites are listed below: (*** & bold = letter of interest provided;** only * = verbal/e-mail statement of interest)

University of Cincinnati

***Procter & Gamble, Phase & Colloid Science Analytic Division (First Membership)**
***LyondelBasell Industries**
***Dupont, Experimental Station, Wilmington, DE**
***Oak Ridge National Laboratory**
***Bridgestone/Firestone**
***Eclipse Film Technologies**
***ThreeBond Corporation**
*Avery Dennison Corporation
*SABIC Americas
DSM Hybrane Division
Goodyear Tire & Rubber
Goodrich Tire
PPG Industries
Nova Chemicals
Ashland Chemicals
Ticona Coporation
PolyOne Corporation

University of Michigan

***ExxonMobil, Baytown, TX (First Membership)**
***Dow Chemical, Freeport TX**
***Air Force Research Laboratory**
***Procter & Gamble Materials Science & Technology (Second Membership)**
***Myaterials**
***Dow Corning Corporation**
*ExxonMobil, Research & Engineering Co. (Second Membership)
*Procter & Gamble, Baby Care Division (Third Membership)
*Sandia National Laboratory
Michigan Molecular Institute
3M Corporation
Soldier Research, Development and Engineering Center (NSRDEC) U. S. Army Natick, MA
Total Petrochemicals
ChevronPhillips

University of Cincinnati Letters

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

February 16, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from my organization. We would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

Michael R. Weaver, Ph.D.
Principal Scientist, Analytical Sciences
Corporate Engineering Technology Labs
Procter & Gamble Co.
8256 Union Center Blvd.
West Chester, OH 45069
weaver.mr@pg.com

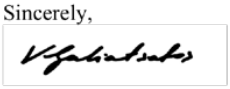
Rathindra (Babu) DasGupta, PhD
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

March 4, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. I have looked through the Planning Grant proposal and other information the PI's have provided concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from my organization. We would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,



Vassilios Galiatsatos, PhD
vassilios.galiatsatos@lyondellbasell.com

Equistar Chemicals, LP
Cincinnati Technology Center
11530 Northlake Drive
Cincinnati, OH 45249
Tel 513-530-4263
lyondellbasell.com

DuPont Central Research & Development
Experimental Station
Wilmington, DE 19880-0323
(302) 695 1222
j-david.londono@usa.dupont.com

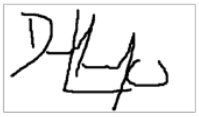
March 4, 2011

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

Dear Dr. DasGupta,

The PI's of the proposed Center for Macromolecular Topology have requested that my organization consider participation in the proposed NSF Center. We continue to look through and discuss the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. We have discussed the Center's concept and proposed research agenda and we will consider their potential for receiving support, particularly if the research directions are guided towards our interests. We intend to attend the Planning Meeting in the Fall of 2011 to discuss the Center and to give input on interesting research directions.

Sincerely,



J D Londono
Senior Research Associate

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Gregory S. Smith
Group Leader, Low Q
Neutron Scattering Science Division
P.O. Box 2008
Oak Ridge, TN 37831-6393
(865) 241-1742
Email: smithgs1@ornl.gov

March 1, 2011

Dr. Gregory Beaucage
Chemical & Materials Engineering Department
RHODES 492
P. O. Box 210012
Cincinnati OH 45221

RE: Letter of Interest in the Proposed I/UCRC Center for Macromolecular Topology

Dear Greg:

I am writing this letter to express my interest in your proposed I/UCRC Center for Macromolecular Topology. Currently, I am the Group Leader for the Low-Q instruments at both HFIR and SNS, two of the highest flux neutron sources in the world. As you know, neutron scattering is one of the most powerful techniques for studying macromolecular structures. Based on my understanding of your proposed idea for the Center, work in my group certainly overlaps with some of your Center's goals. Because of this alignment of our research capabilities and interests with the subject of your proposed Center, I would be interested to attend your planning meeting in the Fall of 2011 to see where neutron scattering might play a unique role in the research activities of the Center.

Sincerely,

Gregory S. Smith

Gregory S. Smith, PhD
Low-Q Group Leader
Neutron Scattering Science Division

Bridgestone Americas
Center for Research and Technology
Mail: 1200 Firestone Parkway
Akron, OH 44317-0001
Ship: 1659 South Main Street
Akron, OH 44301
Phone: 330-379-7000
Fax: 330-379-7530

Rathindra (Babu) DasGupta, PhD
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

March 2, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from my organization. We would give some consideration to joining the Center if it were formed. We would also consider attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

Robert W. Handlos
Vice President
Research

eclipse film technologies

4434 Muhlhauser Road
Suite 200
Hamilton, Ohio 45011
877.275.4800 toll free
513.942.2900 office
513.942.1444 fax
www.eclipsefilmtech.com

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

February 14, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from my organization. We would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

D. Ryan Breese, Ph.D.
Technical Director

ThreeBond

Dr. Rathindra DasGupta

Program Director, I/UCRC Program

The National Science Foundation

4201 Wilson Boulevard,

Arlington VA 22230

March 3, 2011

Dear Dr. DasGupta:

We are really happy to hear that the Center for Macromolecular Topology is being established at the University of Cincinnati under Dr. Gregory Beaucage's leadership.

Macromolecules and their spatial properties are of high interest to ThreeBond International and, specifically at our facility in Cincinnati, for the adhesive bonding for automotive and electronic applications. Our previous collaborations with University of Cincinnati on the characterization of our oligomers (raw materials) and polymers (finished products) have resulted in scientific advancements, several patents and publications. With the establishment of this new center, I believe our collaboration would increase and both institutions will mutually benefit from this.

We are looking forward to finding out more about the new programs in the Center for Macromolecular Topology and to interacting with Dr. Beaucage in the future.

Yours Sincerely,

Serhan Oztemiz, PhD

Product Development Manager

ThreeBond International, Inc.

xx

1134832

University of Michigan Letters

ExxonMobil Research
and Engineering Company
1545 Route 22 East; Clinton Township
Annandale, NJ 08801-3059

ExxonMobil
Research and Engineering

Date: March 4, 2010

From: Andy H. Tsou, ExxonMobil Research and Engineering Company, Clinton, NJ

To: Rathindra (Babu) DasGupta, Ph.D, Program Director, I/UCRC, Division of Industrial Innovation and Partnerships, 4201 Wilson Blvd., Suite 575.07, Arlington, VA

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from my organization. We would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

Andy H. Tsou, PhD
Section Head, Structure and Performance of Organic Materials
Corporate Strategic Research
ExxonMobil Research and Engineering Company

The Dow Chemical Company
2301 N. Brazosport Blvd.
Freeport, Texas 77541-3257
USA

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

February 24, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that The Dow Chemical Company's Plastics Research organization consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from us. We would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

Willem deGroot
The Dow Chemical Company
2301 Brazosport Blvd.
Freeport, Texas 77541
(979) 238-3306
E-Mail: awillem@dow.com

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

17 February 2011

Richard A. Vaia, Ph.D., USAF
Branch Chief, NanoStructured and Biological Materials
Air Force Research Laboratory (AFRL)
AFRL/RXBN, Bldg 654
2941 Hobson Street
Wright-Patterson AFB, OH 45433-7750

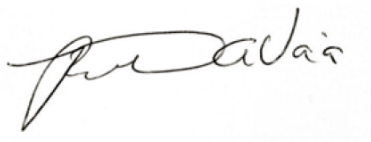
Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

RE: Letter of Interest in the Proposed I/UCRC Center for Macromolecular Topology

Dear Dr. DasGupta,

The Principle Investigators of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda will address scientific challenges underlying numerous programs within my organization. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to provide input into the research directions that would be of interest to my organization.

Sincerely,



Richard A. Vaia, Ph.D., USAF
Branch Chief
Materials and Manufacturing Directorate
Air Force Research Laboratory

P&G

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

March 4, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. I have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. I believe the Center's concept and proposed research agenda have potential for receiving support from my organization. I believe we would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

Isao Noda

Isao Noda, Ph.D., D.Sc.
Research Fellow
Materials Science & Technology
Corporate R&D
The Procter & Gamble Company
8611 Beckett Rd.
West Chester, OH 45069

P&G

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

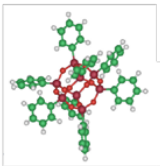
March 4, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that my organization consider participation in the proposed NSF Center. I have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. I believe the Center's concept and proposed research agenda have potential for receiving support from my organization. I believe we would consider joining the Center if it were formed. I am interested in attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to my organization.

Sincerely,

Michael Satkowski, Ph. D
Section Head
Materials Science and Technology
The Procter & Gamble Company
8611 Beckett Rd.
West Chester, OH 45069



Mayaterials Inc.

Silsesquioxane Nano Building Blocks

661 Airport Blvd. Suite 1
Ann Arbor, MI 48104
(734) 994-7035
Mayaterials.com

Dr. Rathindra (Babu) DasGupta,
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

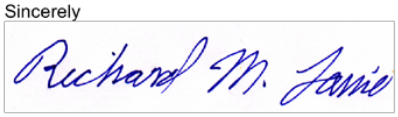
RE: Letter of Interest in Proposed I/UCRC
Center for Macromolecular Topology

Dear Dr. Das Gupta:

Mayaterials has entered its 9th year and has a technology base that relies almost exclusively on the use of diverse silsesquioxane chemistries to develop coating materials for multiple industrial applications. Mayaterials employs some 10 people in Ann Arbor. These silsesquioxanes are macromolecules that place functional groups evenly dispersed around a nanometer sized silica core. These molecules offer 3-D functionality over an extensive range. We believe that the creation of the proposed center would greatly benefit Mayaterials in many ways. First it would provide students that could be hired into our company. Second, it could also serve as a resource center for our company and possibly provide access to analytical tools that we do not have in our current facilities. Third, it would provide an opportunity for a small company to network with other companies.

Consequently, we are wholeheartedly in favor of its formation beginning with the planning grant and look forward to participating in the future.

Sincerely



Richard M. Laine, Ph.D.
CEO

DOW CORNING

Rathindra (Babu) DasGupta, Ph.D
Program Director, I/UCRC
Directorate for Engineering
Division of Industrial Innovation and Partnerships
4201 Wilson Blvd., Suite 575.07
Arlington, VA 22230

March 3, 2011

Dear Dr. DasGupta,

The PI's of the proposed *Center for Macromolecular Topology* have requested that Dow Corning Corporation consider participation in the proposed NSF Center. We have looked through the Planning Grant proposal and other information the PI's have provided to us concerning the proposed I/UCRC Center. The Center's concept and proposed research agenda have the potential for receiving support from my organization and we would consider joining the Center if it were formed. We would also consider attending the Planning Meeting in the Fall of 2011 to discuss the Center and to give input into the research directions that would be of interest to Dow Corning.

Sincerely,

Steven H. Waier

Steven H. Waier
Market Supply Tech Center Manager
Dow Corning Corporation
(989)-496-5806

Dow Corning Corporation
2200 W. Salzburg Rd
P.O. Box 994, #CO2400
Midland, MI 48686-0994