

**02 INFORMATION ABOUT PRINCIPAL INVESTIGATORS/PROJECT DIRECTORS(PI/PD) and  
co-PRINCIPAL INVESTIGATORS/co-PROJECT DIRECTORS**

Submit only ONE copy of this form for each PI/PD and co-PI/PD identified on the proposal. The form(s) should be attached to the original proposal as specified in GPG Section II.C.a. Submission of this information is voluntary and is not a precondition of award. This information will not be disclosed to external peer reviewers. **DO NOT INCLUDE THIS FORM WITH ANY OF THE OTHER COPIES OF YOUR PROPOSAL AS THIS MAY COMPROMISE THE CONFIDENTIALITY OF THE INFORMATION.**

**PI/PD Name:** Gregory Beaucage

**Gender:** ☒ Male ☐ Female

**Ethnicity:** (Choose one response) ☐ Hispanic or Latino ☒ Not Hispanic or Latino

**Race:**  
(Select one or more)

☐ American Indian or Alaska Native  
☐ Asian  
☐ Black or African American  
☐ Native Hawaiian or Other Pacific Islander  
☒ White

**Disability Status:**  
(Select one or more)

☐ Hearing Impairment  
☐ Visual Impairment  
☐ Mobility/Orthopedic Impairment  
☐ Other  
☒ None

**Citizenship:** (Choose one) ☒ U.S. Citizen ☐ Permanent Resident ☐ Other non-U.S. Citizen

**Check here if you do not wish to provide any or all of the above information (excluding PI/PD name):** ☐

**REQUIRED: Check here if you are currently serving (or have previously served) as a PI, co-PI or PD on any federally funded project** ☒

**Ethnicity Definition:**

**Hispanic or Latino.** A person of Mexican, Puerto Rican, Cuban, South or Central American, or other Spanish culture or origin, regardless of race.

**Race Definitions:**

**American Indian or Alaska Native.** A person having origins in any of the original peoples of North and South America (including Central America), and who maintains tribal affiliation or community attachment.

**Asian.** A person having origins in any of the original peoples of the Far East, Southeast Asia, or the Indian subcontinent including, for example, Cambodia, China, India, Japan, Korea, Malaysia, Pakistan, the Philippine Islands, Thailand, and Vietnam.

**Black or African American.** A person having origins in any of the black racial groups of Africa.

**Native Hawaiian or Other Pacific Islander.** A person having origins in any of the original peoples of Hawaii, Guam, Samoa, or other Pacific Islands.

**White.** A person having origins in any of the original peoples of Europe, the Middle East, or North Africa.

**WHY THIS INFORMATION IS BEING REQUESTED:**

The Federal Government has a continuing commitment to monitor the operation of its review and award processes to identify and address any inequities based on gender, race, ethnicity, or disability of its proposed PIs/PDs. To gather information needed for this important task, the proposer should submit a single copy of this form for each identified PI/PD with each proposal. Submission of the requested information is voluntary and will not affect the organization's eligibility for an award. However, information not submitted will seriously undermine the statistical validity, and therefore the usefulness, of information received from others. Any individual not wishing to submit some or all the information should check the box provided for this purpose. (The exceptions are the PI/PD name and the information about prior Federal support, the last question above.)

Collection of this information is authorized by the NSF Act of 1950, as amended, 42 U.S.C. 1861, et seq. Demographic data allows NSF to gauge whether our programs and other opportunities in science and technology are fairly reaching and benefiting everyone regardless of demographic category; to ensure that those in under-represented groups have the same knowledge of and access to programs and other research and educational opportunities; and to assess involvement of international investigators in work supported by NSF. The information may be disclosed to government contractors, experts, volunteers and researchers to complete assigned work; and to other government agencies in order to coordinate and assess programs. The information may be added to the Reviewer file and used to select potential candidates to serve as peer reviewers or advisory committee members. See Systems of Records, NSF-50, "Principal Investigator/Proposal File and Associated Records", 63 Federal Register 267 (January 5, 1998), and NSF-51, "Reviewer/Proposal File and Associated Records", 63 Federal Register 268 (January 5, 1998).

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**PI/PD Name:** Ronald G Larson

**Gender:** ☒ Male ☐ Female

**Ethnicity:** (Choose one response) ☐ Hispanic or Latino ☒ Not Hispanic or Latino

**Race:**  
(Select one or more)

☐ American Indian or Alaska Native  
☐ Asian  
☐ Black or African American  
☐ Native Hawaiian or Other Pacific Islander  
☒ White

**Disability Status:**  
(Select one or more)

☐ Hearing Impairment  
☐ Visual Impairment  
☐ Mobility/Orthopedic Impairment  
☐ Other  
☒ None

**Citizenship:** (Choose one) ☒ U.S. Citizen ☐ Permanent Resident ☐ Other non-U.S. Citizen

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## **List of Suggested Reviewers or Reviewers Not To Include (optional)**

---

### **SUGGESTED REVIEWERS:**

**Prof. Ralph H. Colby**  
Department of Materials Science & Engineering  
The Pennsylvania State University  
309 Steidle Building  
University Park, PA  
(814) 863 - 3457  
rhc@plmsc.psu.edu

**Prof. Jay D. Schieber**  
Chemical and Biological Engineering  
Illinois Institute of Technology  
Perlstein Hall, Suite 127  
10 W. 33rd Street  
Chicago, IL 60616  
(312) 567-3046  
schieber@iit.edu

**Prof. Mort Denn**  
Levich Institute  
City College of New York  
Steinman Hall #1M  
140th Street & Convent Ave  
New York, NY 10031  
(212) 650-7444  
denn@levdec.engr.ccny.cuny.edu

**Prof. Linda S. Schadler**  
Associate Dean for Academic Affairs  
Rensselaer Polytechnical Institute  
JEC 2018  
110 8'th Street  
Troy, NY 12180  
(518) 276-6626  
schadl@rpi.edu

**Prof. Michael Harris**  
Associate Dean of Engineering for Undergraduate Education  
and Professor Department of Chemical Engineering  
Purdue University  
ARMS G051  
Lafayette, IN  
(765) 494-0963  
mtharris@purdue.edu

### **REVIEWERS NOT TO INCLUDE:**

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## List of Suggested Reviewers or Reviewers Not To Include (optional)

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Reviewers not to include contd...

## List of Suggested Reviewers or Reviewers Not To Include (optional)

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### **SUGGESTED REVIEWERS:**

Not Listed

### **REVIEWERS NOT TO INCLUDE:**

Not Listed

## 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					<b>FOR NSF USE ONLY</b>	
<b>NSF 10-595</b>			<b>03/06/11</b>			<b>NSF PROPOSAL NUMBER</b>
FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)						
<b>IIP - INDUSTRY/UNIV COOP RES CENTERS</b>						
DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)		FILE LOCATION
				<b>041064767</b>		
EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)		SHOW PREVIOUS AWARD NO. IF THIS IS <input type="checkbox"/> A RENEWAL <input type="checkbox"/> AN ACCOMPLISHMENT-BASED RENEWAL		IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES <input type="checkbox"/> NO <input checked="" type="checkbox"/> IF YES, LIST ACRONYM(S)		
<b>316000989</b>						
NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE			ADDRESS OF Awardee ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE			
<b>University of Cincinnati Main Campus</b>			<b>University of Cincinnati Main Campus</b>			
AWARDEE ORGANIZATION CODE (IF KNOWN)			<b>University Hall, Suite 530</b>			
<b>0031252000</b>			<b>Cincinnati, OH. 452210222</b>			
NAME OF PRIMARY PLACE OF PERF			ADDRESS OF PRIMARY PLACE OF PERF, INCLUDING 9 DIGIT ZIP CODE			
<b>University of Cincinnati Main Campus</b>			<b>University of Cincinnati Main Campus</b>			
			<b>492 Rhodes Hall</b>			
			<b>Cincinnati ,OH ,452210012 ,US.</b>			
IS Awardee ORGANIZATION (Check All That Apply) (See GPG II.C For Definitions)		<input type="checkbox"/> SMALL BUSINESS <input type="checkbox"/> FOR-PROFIT ORGANIZATION		<input type="checkbox"/> MINORITY BUSINESS <input type="checkbox"/> WOMAN-OWNED BUSINESS		<input type="checkbox"/> IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE
TITLE OF PROPOSED PROJECT <b>Planning Grant: I/UCRC for The Center for Macromolecular Topology (CMT)</b>						
REQUESTED AMOUNT \$ <b>14,500</b>		PROPOSED DURATION (1-60 MONTHS) <b>12</b> months		REQUESTED STARTING DATE <b>09/01/11</b>		SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE
CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW						
<input type="checkbox"/> BEGINNING INVESTIGATOR (GPG I.G.2)			<input type="checkbox"/> HUMAN SUBJECTS (GPG II.D.7) Human Subjects Assurance Number _____			
<input type="checkbox"/> DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C.1.e)			Exemption Subsection _____ or IRB App. Date _____			
<input type="checkbox"/> PROPRIETARY & PRIVILEGED INFORMATION (GPG I.D., II.C.1.d)			<input checked="" type="checkbox"/> INTERNATIONAL COOPERATIVE ACTIVITIES: COUNTRY/COUNTRIES INVOLVED			
<input type="checkbox"/> HISTORIC PLACES (GPG II.C.2.j)			(GPG II.C.2.j) <b>UK</b>			
<input type="checkbox"/> EAGER* (GPG II.D.2) <input type="checkbox"/> RAPID** (GPG II.D.1)			<input type="checkbox"/> HIGH RESOLUTION GRAPHICS/OTHER GRAPHICS WHERE EXACT COLOR REPRESENTATION IS REQUIRED FOR PROPER INTERPRETATION (GPG I.G.1)			
<input type="checkbox"/> VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____						
PHS Animal Welfare Assurance Number _____						
PI/PD DEPARTMENT <b>Materials and Chemical Engineering</b>			PI/PD POSTAL ADDRESS <b>P.O. Box 210012</b>			
PI/PD FAX NUMBER <b>513-556-2569</b>			<b>Cincinnati, OH 452210012</b>			
			<b>United States</b>			
NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address		
<b>Gregory Beaucage</b>	<b>PhD</b>	<b>1991</b>	<b>513-556-3063</b>	<b>beaucag@uc.edu</b>		
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						

## 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.

### Certification Regarding Nondiscrimination

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative is providing the Certification Regarding Nondiscrimination contained in Exhibit II-6 of the Grant Proposal Guide.

### 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.

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative or Individual Applicant located in FEMA-designated special flood hazard areas is certifying that adequate flood insurance has been or will be obtained in the following situations:

- (1) for NSF grants for the construction of a building or facility, regardless of the dollar amount of the grant; and
- (2) for other NSF Grants when more than \$25,000 has been budgeted in the proposal for repair, alteration or improvement (construction) of a building or facility.

### Certification Regarding Responsible Conduct of Research (RCR)

(This certification is not applicable to proposals for conferences, symposia, and workshops.)

By electronically signing the NSF Proposal Cover Sheet, the Authorized Organizational Representative of the applicant institution is certifying that, in accordance with the NSF Proposal & Award Policies & Procedures Guide, Part II, Award & Administration Guide (AAG) Chapter IV.B., the institution has a plan in place to provide appropriate training and oversight in the responsible and ethical conduct of research to undergraduates, graduate students and postdoctoral researchers who will be supported by NSF to conduct research.

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					
TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS			FAX NUMBER	

\* EAGER - Early-concept Grants for Exploratory Research

\*\* RAPID - Grants for Rapid Response Research

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NSF 10-595 03/06/11					NSF PROPOSAL NUMBER	
FOR CONSIDERATION BY NSF ORGANIZATION UNIT(S) (Indicate the most specific unit known, i.e. program, division, etc.)						
IIP - INDUSTRY/UNIV COOP RES CENTERS						
DATE RECEIVED	NUMBER OF COPIES	DIVISION ASSIGNED	FUND CODE	DUNS# (Data Universal Numbering System)	FILE LOCATION	
				073133571		
EMPLOYER IDENTIFICATION NUMBER (EIN) OR TAXPAYER IDENTIFICATION NUMBER (TIN)		SHOW PREVIOUS AWARD NO. IF THIS IS <input type="checkbox"/> A RENEWAL <input type="checkbox"/> AN ACCOMPLISHMENT-BASED RENEWAL		IS THIS PROPOSAL BEING SUBMITTED TO ANOTHER FEDERAL AGENCY? YES <input type="checkbox"/> NO <input checked="" type="checkbox"/> IF YES, LIST ACRONYM(S)		
386006309						
NAME OF ORGANIZATION TO WHICH AWARD SHOULD BE MADE University of Michigan Ann Arbor			ADDRESS OF Awardee ORGANIZATION, INCLUDING 9 DIGIT ZIP CODE 3003 South State St. Room 1062 Ann Arbor, MI 48109-1271			
AWARDEE ORGANIZATION CODE (IF KNOWN) 0023259000						
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)		<input type="checkbox"/> SMALL BUSINESS <input type="checkbox"/> FOR-PROFIT ORGANIZATION		<input type="checkbox"/> MINORITY BUSINESS <input type="checkbox"/> WOMAN-OWNED BUSINESS		<input type="checkbox"/> IF THIS IS A PRELIMINARY PROPOSAL THEN CHECK HERE
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REQUESTED AMOUNT \$ 11,499	PROPOSED DURATION (1-60 MONTHS) 12 months		REQUESTED STARTING DATE 09/01/11		SHOW RELATED PRELIMINARY PROPOSAL NO. IF APPLICABLE	
CHECK APPROPRIATE BOX(ES) IF THIS PROPOSAL INCLUDES ANY OF THE ITEMS LISTED BELOW <input type="checkbox"/> BEGINNING INVESTIGATOR (GPG I.G.2) <input type="checkbox"/> DISCLOSURE OF LOBBYING ACTIVITIES (GPG II.C.1.e) <input type="checkbox"/> PROPRIETARY & PRIVILEGED INFORMATION (GPG I.D, II.C.1.d) <input type="checkbox"/> HISTORIC PLACES (GPG II.C.2.j) <input type="checkbox"/> EAGER* (GPG II.D.2) <input type="checkbox"/> RAPID** (GPG II.D.1) <input type="checkbox"/> VERTEBRATE ANIMALS (GPG II.D.6) IACUC App. Date _____ PHS Animal Welfare Assurance Number _____						
PI/PD DEPARTMENT Chemical Engineering			PI/PD POSTAL ADDRESS 2300 Hayward, 3074 H.H. Dow Bldg.  Ann Arbor, MI 481092136 United States			
PI/PD FAX NUMBER 734-763-0459						
NAMES (TYPED)	High Degree	Yr of Degree	Telephone Number	Electronic Mail Address		
PI/PD NAME Ronald G Larson	PhD	1980	734-936-0772	rlarson@umich.edu		
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						
CO-PI/PD						



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Yes ☐

No ☒

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- (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.
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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					
TELEPHONE NUMBER	ELECTRONIC MAIL ADDRESS			FAX NUMBER	

\* 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 National 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.

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## 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 Corporation  
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)  
\*Materials  
\*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 Supplemental 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 from 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,  $\phi_{Br}$ , 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,  $\phi_{si}$  [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.

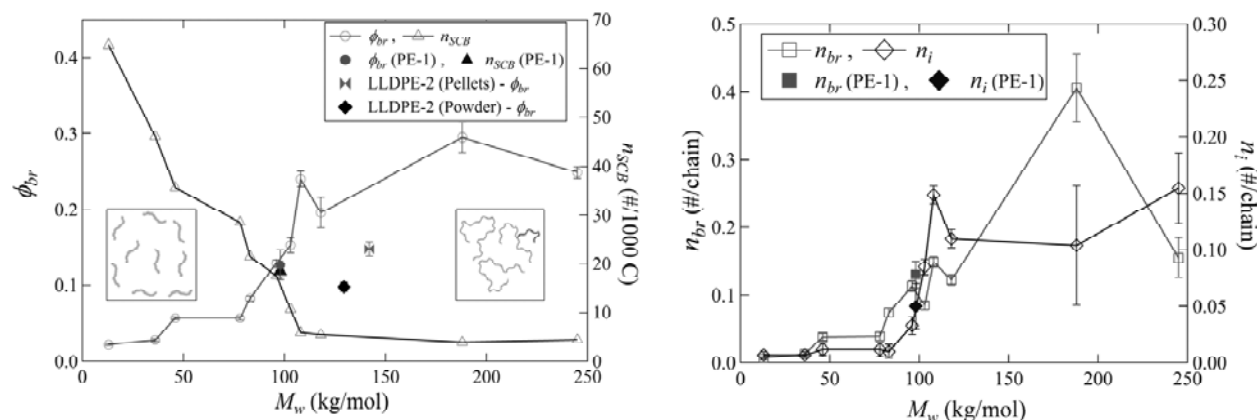


Figure 1. a) Plot of mole-fraction LCB content,  $\phi_{br}$ , from equation (7) and number of SCBs per 1000 Carbon atoms,  $n_{SCB}$ , from NMR against the weight-average molecular weight,  $M_w$ , obtained from SANS [8]. b) Plot of number of LCB sites per chain,  $n_{br}$ , from equation (9) and number 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 a promising young macromolecular scientists are expected to participate in the Center at the University of Michigan site. Prof. Rick Laine is well known 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.

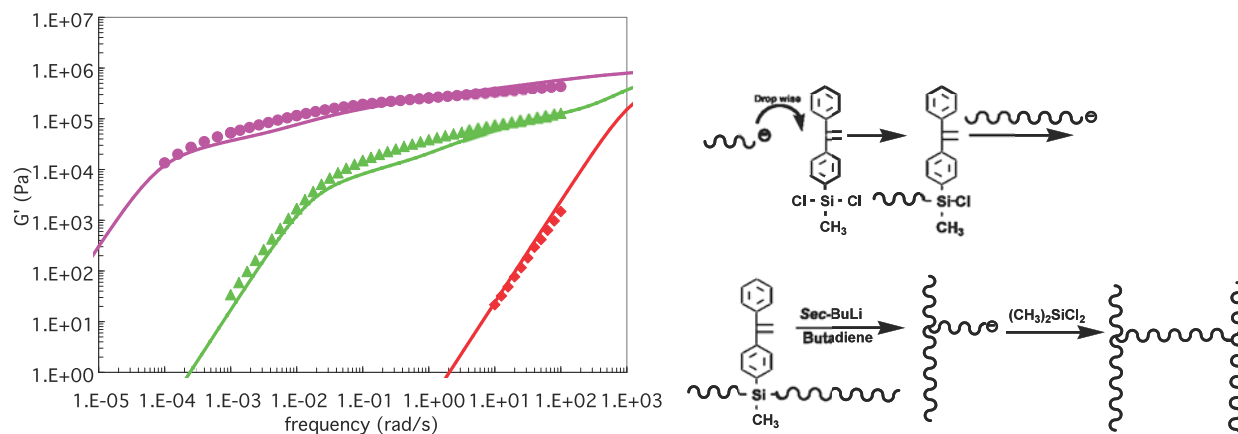
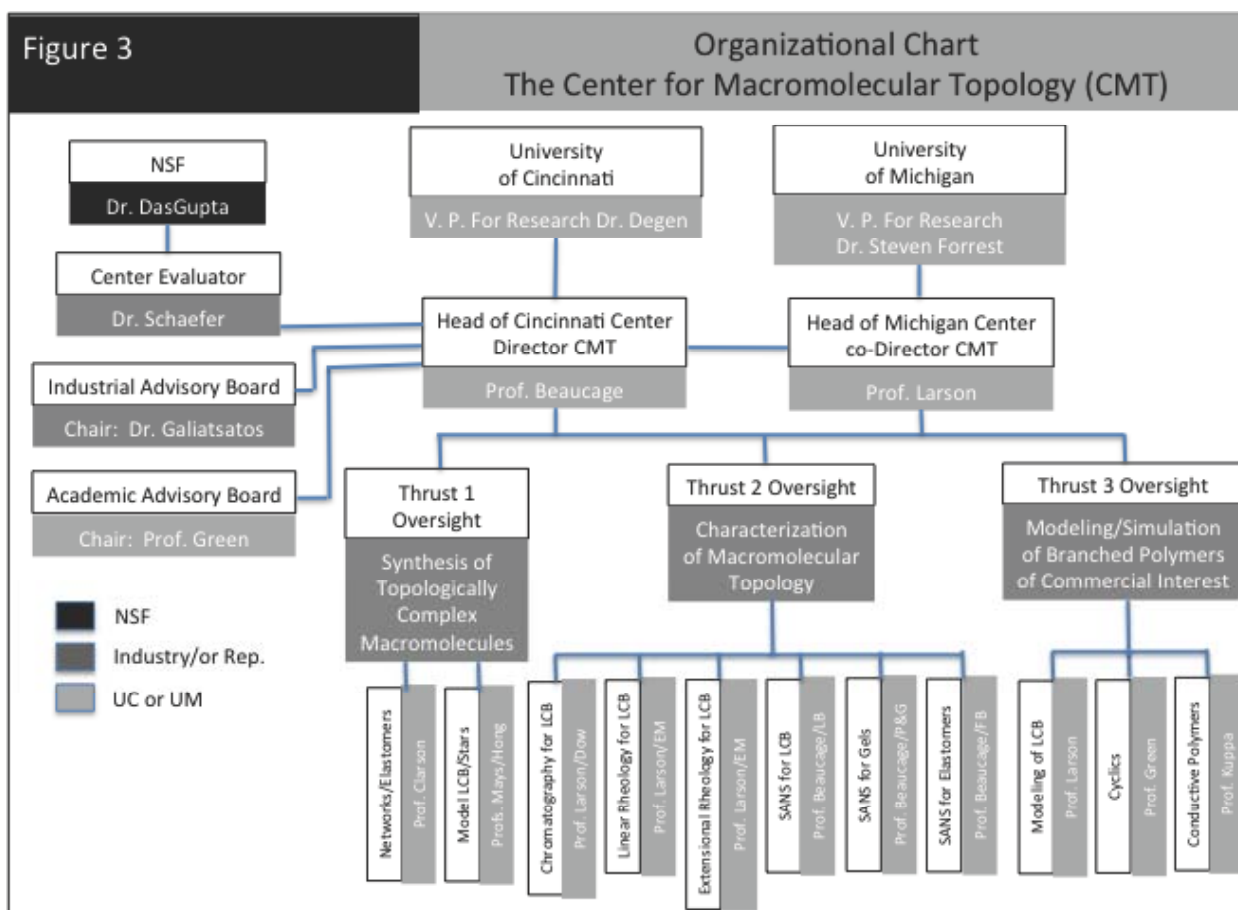


Figure 2. (a) Storage modulus of “H” polymer (violet), linear-shaped (red), and a 50-50 blend (green), all of polybutadiene. Lines are calculations based on Larson’s hierarchical model and points are experimental measurements. (b) An example of a synthetic scheme for making monodisperse asymmetric H-PBd 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 used by P&G in the manufacture of diapers and other consumer products. These materials are also used 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:* Superabsorbent samples, provided by Procter & Gamble, will be swollen in D<sub>2</sub>O 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 superabsorbent 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.

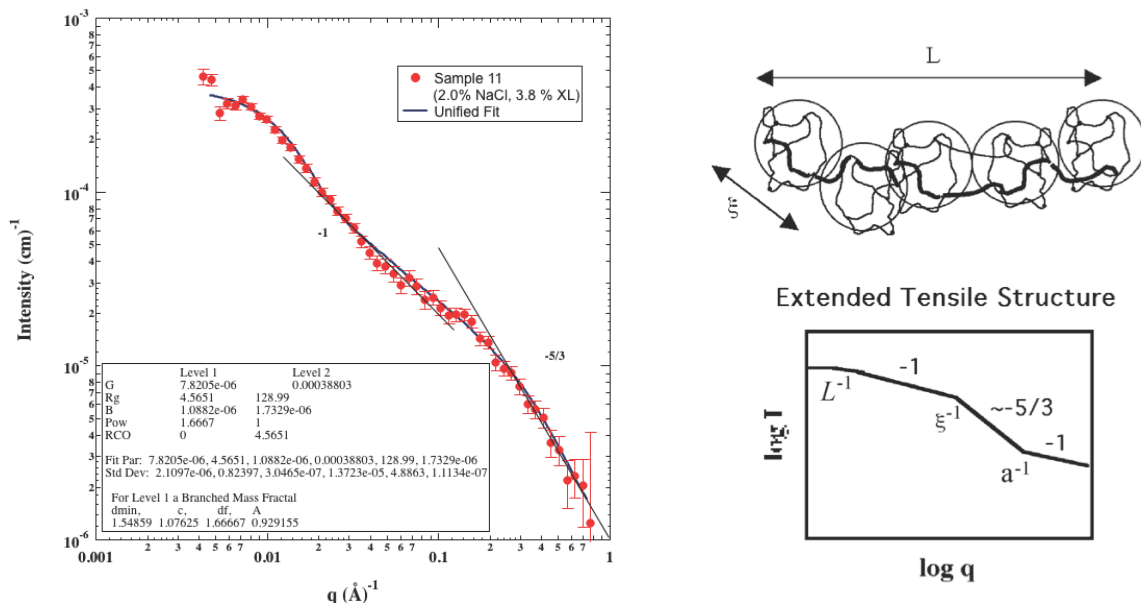


Figure 7. (a) Preliminary data from ORNL/HFIR facility on a PAA gel with 3.8 % cross linker concentration and swollen in a 2% salt solution. The fit is to the GTB model and reflects a mesh size of 44.7 nm with a tensile structural transition at 2.1 nm. The data also contains information concerning the 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. Kuppia, 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. Kuppia 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 the 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, 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, will 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 it is 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 titania 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 Rheology 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 Kuppala (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 a collaboration with Jimmy Mays of the University of Tennessee, and his lab to produce 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 a 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 both 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 Zurich 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<sub>2</sub> 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 than 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<sub>2</sub> 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<sub>2</sub>. The effects of catalyst support structure in the DP method were studied using TiO<sub>2</sub> produced in SFP of variable morphology. The activity of catalysts prepared using the flame made TiO<sub>2</sub> is even higher than the catalysts made using commercial TiO<sub>2</sub>. 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.* 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**(5) 2005 (Article 054309).
- 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.* 2002 59 714–720.
- 14) *Neutron scattering from equilibrium-swollen networks.* Sukumaran SK, Beaucage G., Mark JE, Viers, B. *Eur. Phys. J. E* 2005 18 29–36.
- 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 (2004a).

- 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**(5) 054309 (2005).
- 21) *Determination of branch fraction and minimum dimension of mass-fractal aggregates.* Beaucage G, *Phys. Rev. E*, **70**, 031401 (2004c).
- 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).

## Gregory Beaucage, Professor

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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 National Laboratory.

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,

# SUMMARY PROPOSAL BUDGET

YEAR 1

ORGANIZATION <b>University of Cincinnati Main Campus</b>				FOR NSF USE ONLY			
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR <b>Gregory Beaucage</b>				PROPOSAL NO.	DURATION (months)		
				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1. <b>Gregory Beaucage - Professor</b>				0.00	0.00	0.23	\$ 2,631
2.							
3.							
4.							
5.							
6. ( 0 ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. ( 1 ) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.23	2,631
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. ( 0 ) POST DOCTORAL SCHOLARS				0.00	0.00	0.00	0
2. ( 0 ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00	0
3. ( 0 ) GRADUATE STUDENTS							0
4. ( 0 ) UNDERGRADUATE STUDENTS							0
5. ( 0 ) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							0
6. ( 0 ) OTHER							0
TOTAL SALARIES AND WAGES (A + B)							2,631
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							805
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							3,436
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							500
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ 0							
2. TRAVEL 0							
3. SUBSISTENCE 0							
4. OTHER 0							
TOTAL NUMBER OF PARTICIPANTS ( 0 ) TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							0
3. CONSULTANT SERVICES							3,000
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							2,300
TOTAL OTHER DIRECT COSTS							5,300
H. TOTAL DIRECT COSTS (A THROUGH G)							9,236
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) <b>Modified Total Direct Cost (MTDC) (Rate: 57.0000, Base: 9235)</b>							
TOTAL INDIRECT COSTS (F&A)							5,264
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							14,500
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 14,500
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME <b>Gregory Beaucage</b>				FOR NSF USE ONLY			
ORG. REP. NAME*				INDIRECT COST RATE VERIFICATION			
				Date Checked	Date Of Rate Sheet	Initials - ORG	

1 \*ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

# SUMMARY PROPOSAL BUDGET

Cumulative

ORGANIZATION <b>University of Cincinnati Main Campus</b>				FOR NSF USE ONLY			
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR <b>Gregory Beaucage</b>				PROPOSAL NO.	DURATION (months)		
				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1. <b>Gregory Beaucage - Professor</b>				0.00	0.00	0.23	\$ 2,631
2.							
3.							
4.							
5.							
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. ( <b>1</b> ) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.23	2,631
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. ( <b>0</b> ) POST DOCTORAL SCHOLARS				0.00	0.00	0.00	0
2. ( <b>0</b> ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00	0
3. ( <b>0</b> ) GRADUATE STUDENTS							0
4. ( <b>0</b> ) UNDERGRADUATE STUDENTS							0
5. ( <b>0</b> ) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							0
6. ( <b>0</b> ) OTHER							0
TOTAL SALARIES AND WAGES (A + B)							2,631
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							805
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							3,436
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							500
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ _____							0
2. TRAVEL _____							0
3. SUBSISTENCE _____							0
4. OTHER _____							0
TOTAL NUMBER OF PARTICIPANTS ( <b>0</b> ) TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							0
3. CONSULTANT SERVICES							3,000
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							2,300
TOTAL OTHER DIRECT COSTS							5,300
H. TOTAL DIRECT COSTS (A THROUGH G)							9,236
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)							
TOTAL INDIRECT COSTS (F&A)							5,264
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							14,500
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 14,500
M. COST SHARING PROPOSED LEVEL \$ <b>0</b>				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME <b>Gregory Beaucage</b>				FOR NSF USE ONLY			
ORG. REP. NAME*				INDIRECT COST RATE VERIFICATION			
				Date Checked	Date Of Rate Sheet	Initials - ORG	

C \*ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

## **Budget Justification**

### **SALARIES**

The proposed budget includes ~1 week recess effort by the PI (\$2631).

### **FRINGE**

Fringe Benefits are a direct-charge as a percentage of salaries and wages at rates established by the university, and reviewed annually by DHHS, for salary expenses.

### **TRAVEL**

The I/UCRC program requires attendance at an NSF “Boot Camp”. \$500 in travel is allocated for this trip and for travel to the Center site at the University of Michigan for planning of the project.

### **OTHER DIRECT COSTS**

\$2,300 is allocated for the planning meeting. This is the estimated cost for rental of a meeting space at the Kingsgate Conference Center on the University of Cincinnati Campus (\$500) and two breakfasts, lunch and one dinner for 50 attendees with 24% for service and 6.5% for tax. The estimated attendees include 36 company and national lab representatives, 1 NSF representative, 5 representatives from the University of Cincinnati and 5 representatives from the University of Michigan.

\$3,000 is allocated as a consultancy to the Center evaluator. This will be paid in a lump sum payment for all services associated with planning the Center.

### **INDIRECT COSTS**

Indirect costs are charged at 57.0% of Modified Total Direct Costs (MTDC) per DHHS rate agreement dated 04/01/10, excluding equipment, and tuition.

# SUMMARY PROPOSAL BUDGET

YEAR 1

ORGANIZATION				FOR NSF USE ONLY		
<b>University of Michigan Ann Arbor</b>				PROPOSAL NO.		DURATION (months)
						Proposed      Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR <b>Ronald G Larson</b>				AWARD NO.		
A. SENIOR PERSONNEL: PI/PI, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer
				CAL	ACAD	SUMR
1. <b>Ronald G Larson - Project Investigator</b>				0.00	0.00	0.12 \$ 3,222
2.						
3.						
4.						
5.						
6. ( 0 ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00 0
7. ( 1 ) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.12 3,222
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( 0 ) POST DOCTORAL SCHOLARS				0.00	0.00	0.00 0
2. ( 0 ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00 0
3. ( 0 ) GRADUATE STUDENTS						0
4. ( 0 ) UNDERGRADUATE STUDENTS						0
5. ( 0 ) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)						0
6. ( 0 ) OTHER						0
TOTAL SALARIES AND WAGES (A + B)						3,222
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)						967
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)						4,189
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)						
TOTAL EQUIPMENT						0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)						3,206
2. FOREIGN						0
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS \$ 0						
2. TRAVEL 0						
3. SUBSISTENCE 0						
4. OTHER 0						
TOTAL NUMBER OF PARTICIPANTS ( 0 ) TOTAL PARTICIPANT COSTS						0
G. OTHER DIRECT COSTS						
1. MATERIALS AND SUPPLIES						0
2. PUBLICATION COSTS/DOCUMENTATION/DISEMINATION						0
3. CONSULTANT SERVICES						0
4. COMPUTER SERVICES						0
5. SUBAWARDS						0
6. OTHER						0
TOTAL OTHER DIRECT COSTS						0
H. TOTAL DIRECT COSTS (A THROUGH G)						7,395
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE) <b>Modified Total Direct Cost (MTDC) (Rate: 55.5000, Base: 7395)</b>						
TOTAL INDIRECT COSTS (F&A)						4,104
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)						11,499
K. RESIDUAL FUNDS						0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)						\$ 11,499 \$
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$		
PI/PI NAME				FOR NSF USE ONLY		
<b>Ronald G Larson</b>				INDIRECT COST RATE VERIFICATION		
ORG. REP. NAME*				Date Checked	Date Of Rate Sheet	Initials - ORG

1 \*ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

# SUMMARY PROPOSAL BUDGET

Cumulative

ORGANIZATION <b>University of Michigan Ann Arbor</b>				FOR NSF USE ONLY			
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR <b>Ronald G Larson</b>				PROPOSAL NO.	DURATION (months)		
				AWARD NO.	Proposed	Granted	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates (List each separately with title, A.7. show number in brackets)				NSF Funded Person-months		Funds Requested By proposer	Funds granted by NSF (if different)
				CAL	ACAD	SUMR	
1. <b>Ronald G Larson - Project Investigator</b>				0.00	0.00	0.12	\$ 3,222
2.							
3.							
4.							
5.							
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAGE)				0.00	0.00	0.00	0
7. ( 1 ) TOTAL SENIOR PERSONNEL (1 - 6)				0.00	0.00	0.12	3,222
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. ( 0 ) POST DOCTORAL SCHOLARS				0.00	0.00	0.00	0
2. ( 0 ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				0.00	0.00	0.00	0
3. ( 0 ) GRADUATE STUDENTS							0
4. ( 0 ) UNDERGRADUATE STUDENTS							0
5. ( 0 ) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)							0
6. ( 0 ) OTHER							0
TOTAL SALARIES AND WAGES (A + B)							3,222
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)							967
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)							4,189
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEEDING \$5,000.)							
TOTAL EQUIPMENT							0
E. TRAVEL 1. DOMESTIC (INCL. CANADA, MEXICO AND U.S. POSSESSIONS)							3,206
2. FOREIGN							0
F. PARTICIPANT SUPPORT COSTS							
1. STIPENDS \$ 0							0
2. TRAVEL 0							0
3. SUBSISTENCE 0							0
4. OTHER 0							0
TOTAL NUMBER OF PARTICIPANTS ( 0 ) TOTAL PARTICIPANT COSTS							0
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES							0
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION							0
3. CONSULTANT SERVICES							0
4. COMPUTER SERVICES							0
5. SUBAWARDS							0
6. OTHER							0
TOTAL OTHER DIRECT COSTS							0
H. TOTAL DIRECT COSTS (A THROUGH G)							7,395
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)							
TOTAL INDIRECT COSTS (F&A)							4,104
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)							11,499
K. RESIDUAL FUNDS							0
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)							\$ 11,499
M. COST SHARING PROPOSED LEVEL \$ 0				AGREED LEVEL IF DIFFERENT \$			
PI/PD NAME <b>Ronald G Larson</b>				FOR NSF USE ONLY			
ORG. REP. NAME*				INDIRECT COST RATE VERIFICATION			
				Date Checked	Date Of Rate Sheet	Initials - ORG	

C \*ELECTRONIC SIGNATURES REQUIRED FOR REVISED BUDGET

## **Budget Justification for NSF sponsored boot camp**

### **A. Senior Personnel:**

PI: Ronald Larson, Ph.D., Professor, Chemical Engineering, University of Michigan is requesting 0.125 summer month salary. The University of Michigan faculty salaries are based on 2010-11 rates, incremented for anticipated cost of living and other adjustments. An annual escalation factor of 4% has been used based on past year increases.

### **B. Other Personnel:**

No other salary is requested.

### **C. Fringe Benefits:**

Fringe benefits have been calculated at 30% for Senior Personnel.

### **D. Equipment:**

No equipment is requested.

### **E. Travel:**

Domestic Travel has been estimated based on sample flight costs and daily expense rates for general domestic destinations. It is estimated for five trips. One trip each for Larson, a University of Michigan administrator (Dept chair or higher) and a student to attend a fall planning workshop where the full proposal will be presented. In addition, Larson requests funds for two additional trips to Cincinnati to meet with Greg Beaucage for planning details of the grant.

### **F. Participant Support Costs:**

No participant support costs requested.

### **G. Other Direct Costs:**

No other costs requested.

### **I. Indirect Costs:**

Overhead for this project has been calculated at the same F&A rate established at University of Michigan. This rate is currently 55.5%. The modified total direct cost base (MTDC) amount used in calculating the indirect costs is the total direct costs, excluding capital equipment, graduate student tuition, participant costs and individual subcontract amounts in excess of \$25,000.

## Current and Pending Support

(See GPG Section II.C.2.h for guidance on information to include on this form.)

The following information should be provided for each investigator and other senior personnel. Failure to provide this information may delay consideration of this proposal.	
Investigator: <b>Gregory Beaucage</b>	Other agencies (including NSF) to which this proposal has been/will be submitted.

Support: <input type="checkbox"/> Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:    Planning Grant: I/UCRC for The Center for Macromolecular Topology (CMT)
Source of Support:    National Science Foundation Total Award Amount: \$    14,500 Total Award Period Covered:    09/01/11 - 08/31/12 Location of Project:    University of Cincinnati Person-Months Per Year Committed to the Project.    Cal:0.00    Acad: 0.00    Sumr: 0.25

Support: <input type="checkbox"/> Current <input checked="" type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:    Materials World Network: Understanding structure/property relationships in nanoparticle aggregates for solar cells in sub-Saharan Africa.
Source of Support:    National Science Foundation Total Award Amount: \$    464,895 Total Award Period Covered:    06/01/11 - 05/31/14 Location of Project:    University of Cincinnati Person-Months Per Year Committed to the Project.    Cal:0.00    Acad: 0.00    Sumr: 0.19

Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:    Quantification of Branch Structure in Polyolefins
Source of Support:    ExxonMobil Corporation Total Award Amount: \$    20,000 Total Award Period Covered:    06/01/10 - 06/01/11 Location of Project:    University of Cincinnati Person-Months Per Year Committed to the Project.    Cal:0.00    Acad: 0.00    Sumr: 0.00

Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:    Characterization of Polyethylene
Source of Support:    LyondellBasell Total Award Amount: \$    75,000 Total Award Period Covered:    04/01/11 - 03/31/12 Location of Project:    University of Cincinnati Person-Months Per Year Committed to the Project.    Cal:0.00    Acad: 1.00    Sumr: 0.00

Support: <input checked="" type="checkbox"/> Current <input type="checkbox"/> Pending <input type="checkbox"/> Submission Planned in Near Future <input type="checkbox"/> *Transfer of Support Project/Proposal Title:    NanoPower Africa
Source of Support:    U.S. Agency for International Development (U.S. State Dept.) Total Award Amount: \$    1,100,000 Total Award Period Covered:    09/01/10 - 12/31/13 Location of Project:    Cincinnati/Cape Town/Oak Ridge/Argonne Person-Months Per Year Committed to the Project.    Cal:0.00    Acad: 2.00    Summ: 1.00

\*If this project has previously been funded by another agency, please list and furnish information for immediately preceding funding period.



## Current and Pending Support

Investigator: Ronald G. Larson

### Current Support:

Project/Proposal Title: Training Grant for Ph.D. Students in the Complex Fluids Area (Co-PI; PI: S. Glotzer)  
Source of Support: Department of Education  
Total Award Amount: \$383,643 (rgl share: \$0)  
Total Award Period Covered: 01/01/07 – 08/31/11  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0      Acad: 0      Sumr: 0

Project/Proposal Title: Synthesis and Rheology of Strategically-Designed Long-Chain-Branched Polymers (PI)  
Source of Support: National Science Foundation  
Total Award Amount: \$399,664  
Total Award Period Covered: 09/01/09 – 08/31/13  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0      Acad: 0      Sumr: 1.0

Project/Proposal Title: Towards a Molecular-Scale Understanding of Flow-Induced Gelation in Thread-Like Micelle Solutions (PI)  
Source of Support: National Science Foundation  
Total Award Amount: \$291,875  
Total Award Period Covered: 05/01/09 – 04/30/12  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0      Acad: 0      Sumr: 0.5

Project/Proposal Title: EFRI-Engineering Synthetic Mimics of DNA-Protein Recognition Systems (PI)  
Source of Support: National Science Foundation  
Total Award Amount: \$1,999,926  
Total Award Period Covered: 05/01/09 – 04/30/12  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0      Acad: 0      Sumr: 0.5

Project/Proposal Title: Reconfigurable Matter from Programmable Colloids (PI: S. Glotzer)  
Source of Support: MURI/DOD – Department of the Army  
Total Award Amount: \$3,750,000  
Total Award Period Covered: 10/01/10 – 9/30/13  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0      Acad: 0.9      Sumr: 0

Pending Support:

Project/Proposal Title: REU Site for Molecular Engineering – Application in Energy and Health (PI: O. Eniola-Adefeso)  
Source of Support: National Science Foundation  
Total Award Amount: \$334,206  
Total Award Period Covered: 05/01/10 – 4/30/13  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0 Acad: 0 Sumr: 0

Project/Proposal Title: Planning Grant: I/UCRC for The Center for Macromolecular Topology (CMT)  
Multiple PI with Gregory Beaucage-Univ. of Cincinnati  
(This Proposal)  
Source of Support: National Science Foundation  
Total Award Amount: \$11,499  
Total Award Period Covered: 09/01/11 – 8/31/12  
Location of Project: Univ. of Michigan, Ann Arbor, MI  
Person-Months Per Year Committed to the Project: Cal: 0 Acad: 0 Sumr: 0.1

## 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<sup>2</sup> 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 Technology and Collin GmbH ([http://www.drcollin.de/en/index\\_en.html](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/Courses/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](http://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: Rheometrics 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<sub>2</sub> 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<sup>rd</sup> floor of the Engineering Research Center has a CM-20 TEM, with a LaB<sub>6</sub> 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 of \$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 compiled, 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 affiliate 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 from 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**

<b>Item</b>	<b>Page</b>
<b>Marketing Plan</b>	<b>ii</b>
<b>Staffing Plan</b>	<b>iv</b>
<b>Draft Industrial Agreement</b>	<b>vi</b>
<b>Draft Association Agreement</b>	<b>viii</b>
<b>Draft Planning Meeting Agenda</b>	<b>x</b>
<b>List of Letters</b>	<b>xii</b>
<b>University of Cincinnati Letters</b>	<b>xiii</b>
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## 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) Specialty applications of macromolecular topology in a variety of situations of use commercially and for the military; 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.

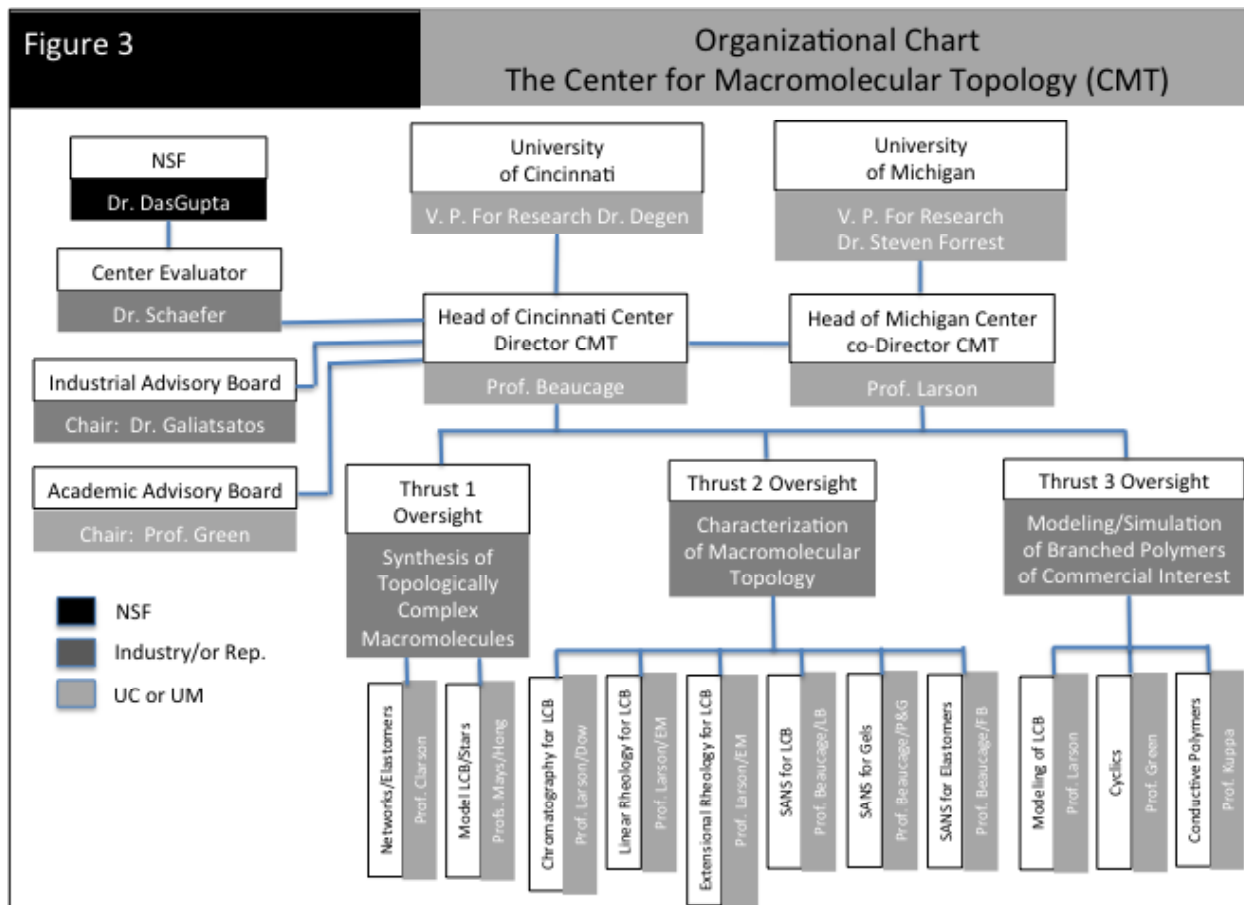
*Center Growth:* It is expected that the center will add two companies per year as full members in the first five years with an attrition rate of one company per 3 years (at the end of a typical project). If the Center begins with 8 full members the center could grow to 15 or 16 members after 5 years 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

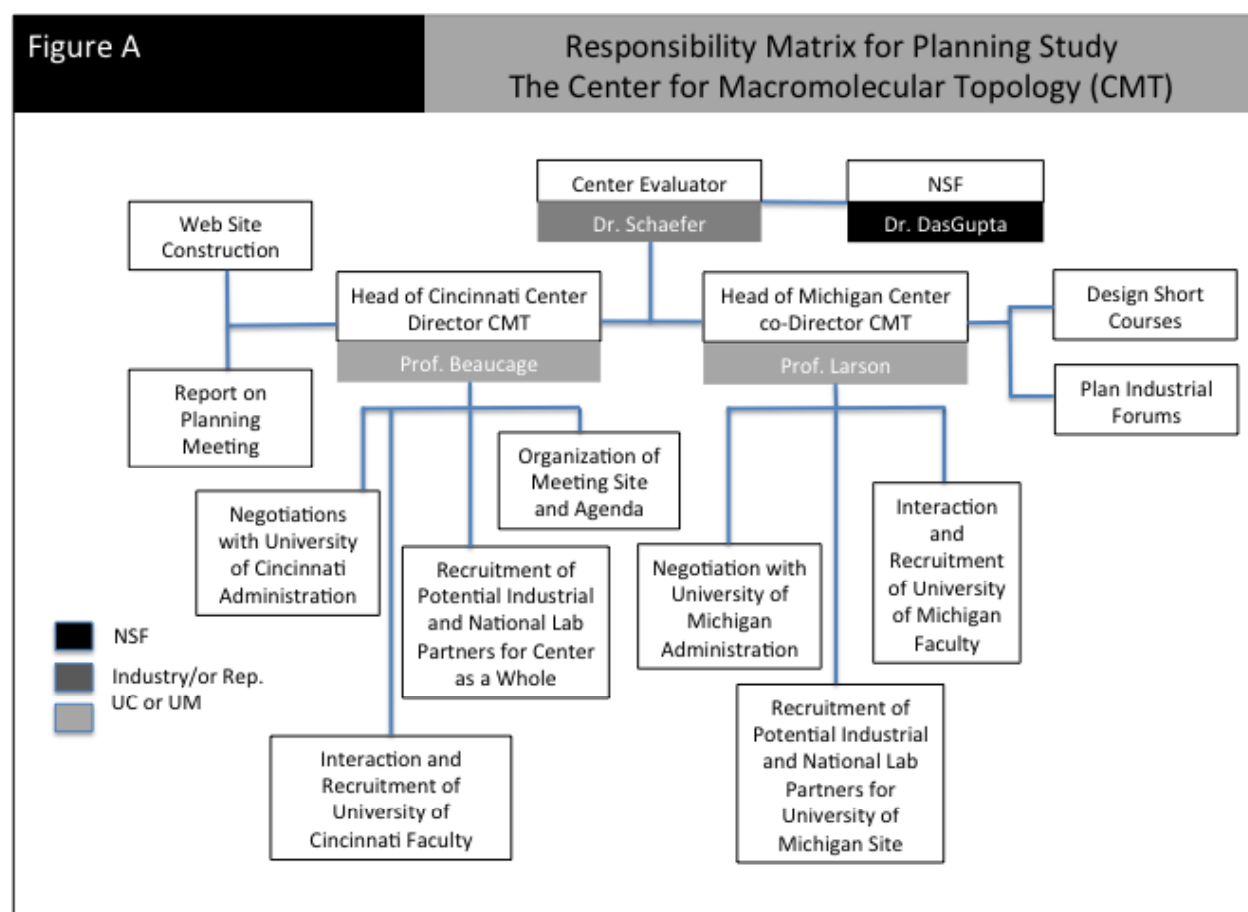
Figure 3 from the Project Description (reproduced below) shows the proposed Organization Chart for the Center for Macromolecular Topology (CMT).



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 Matrix 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.



## **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	<b>BREAK</b>
10:15 - 12:15 pm	<b>Project Presentations (University of Cincinnati)</b> 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	<b>LUNCH</b>
1:00 - 3:00 pm	<b>Project Presentations (University of Michigan)</b> 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	<b>BREAK</b>
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

**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 Corporation  
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,

A handwritten signature in black ink, appearing to read 'M. Weaver'.

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](mailto: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,

A handwritten signature in black ink, appearing to read "V. Galiatsatos", enclosed in a rectangular box.

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,

A handwritten signature in black ink, appearing to read "J D Londono", enclosed within a rectangular box.

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, 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



4434 Muhlbauer Road  
Suite 200  
Hamilton, Ohio 45011  
877.275.4800 toll free  
513.942.2900 office  
513.942.1444 fax  
[www.eclipsefilmtch.com](http://www.eclipsefilmtch.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,

A handwritten signature in dark ink, appearing to read "D. Ryan Breese".

D. Ryan Breese, Ph.D.

Technical Director



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,

A handwritten signature in blue ink, appearing to read "Serhan Oztemiz", with a stylized flourish at the end.

Serhan Oztemiz, PhD  
Product Development Manager  
ThreeBond International, Inc.

**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

An ExxonMobil Subsidiary





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



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,

A handwritten signature in cursive script, reading 'Isao Noda', is positioned above the typed name and title.

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



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

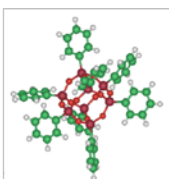
Dear Dr. DasGupta,

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,

A handwritten signature in black ink, which appears to read 'Michael Satkowski'.

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 9<sup>th</sup> 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



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,

A handwritten signature in cursive script that reads "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