

# Newsletter of the LSU Macromolecular Studies Group

Spring 2003

## What's New?- from Paul Russo, Kerry Dooley and Bill Daly, co-directors

### CMC-IGERT



We are still adapting to the \$2.7 Million IGERT grant from the National Science Foundation. IGERT stands for Integrative Graduate Education Research Training.

Across the United States and in all scientific disciplines, there are only 100 IGERT sites. Only a few universities offer IGERT's devoted to polymers and biopolymers. About 20 students in 6 departments have participated as LSU IGERT Fellows. They get a graduate experience limited only by their own imagination. All IGERT sites must propose a new graduate educational model. At LSU, we designed an Apprentice-Artisan-Craftsperson ladder, in which students work very closely with the faculty who are, in turn, a little less constrained because of the ready funding. Ph.D. participants (we call them craftpersons) are requested to spend considerable time with their young student apprentices, working side-by-side with them in the laboratory (or computer terminal, as the case may be). Several professors are finding that working at national or international labs is a good way to meet this responsibility. IGERT teams have made extended visits to the Stanford Synchrotron Radiation Laboratory in California, the Naval

Research Laboratories near Washington DC, and the Laboratorio Nacional de Luz Sincrotron in Brazil. Most of these visits are designed to train LSU students in small angle X-ray scattering and related methods. A new SAXS instrument is being constructed at LSU's synchrotron light source, CAMD. The first scattering patterns were recorded just weeks ago.

In October of 2002, we welcomed a distinguished review panel, and we are busy implementing their suggestions. A common request by the students is more opportunities for industrial co-ops and internships. Please let us know if you're interested. You will find IGERT students adept at working within team environments, but the program also stresses individual performance and creativity.

The IGERT program and other developments within MSG are helping us attract excellent students, but as usual we include recruiting materials to ensure that remains true. *Please post the enclosed color flyer in a conspicuous space.*

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## Professor Thomas Cleij

Thomas Cleij joined the Department of Chemical Engineering in 2000. As a polymer researcher at the interface of science and engineering, he is interested in the development and applications of novel conductive polymers, polymer derived ceramics and polymeric nanocomposites. Thomas obtained his Ph.D. in the Netherlands at Utrecht University (Ph.D. in Physical Organic Chemistry, 1999). His research on novel  $\sigma$ -conjugated conductive polymers and the study of their physical properties led to development of the first water-soluble non-ionic polysilanes and polysilynes. In 1999, he joined U-Cat B.V. in the Netherlands, a

start-up company focusing on applied catalysis and engineering solutions.

Thomas' current research is focused on several areas of applied polymer science and engineering, with an emphasis on hybrid organic-inorganic polymers. Typical examples include the use of  $\sigma$ -conjugated polymers to develop conductive polymer based biosensors, the development of thin ceramic catalyst adhesion layers from polymeric precursors, and the development of carbon nanotubes for integration in polymeric nanocomposites. Additional work focuses on the response of the backbone



conformation of conductive polymers to external stimuli such as temperature, pressure and the polarity and viscosity of the surrounding medium. The research group consists of

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## Personnel Changes

Ben McCoy has joined the Chemical Engineering Department as the first Gordon A. and Mary Cain Chaired Professor. Ben holds degrees from the Illinois Institute of Technology and the University of Minnesota. He came to LSU from the University of California—Davis. His interests include polymer reactions, phase transitions, kinetics and transport.

Marcia Newcomer moved to LSU from Vanderbilt University. She is appointed as Professor in two departments, Chemistry and Biological Sciences. She holds degrees from the College of Charleston and Rice University, and her interests are in protein crystallography. A new beamline at LSU's CAMD synchrotron source is devoted to these studies.

Robert L. Cook is a new assistant professor of chemistry. Following studies at the University of Concordia and the University of Calgary, he did postdocs at Nova Chemicals and the University of Calgary. His interests are in organic matter as found in the natural environment. To this end, he applies sophisticated spectroscopic tools to a variety of macromolecular substances. He is jointly appointed at LSU and Southern University.

Mark McLaughlin accepted a new position as Professor of Chemistry and Interdisciplinary Oncology at the University of South Florida. There, he can continue his novel studies of synthetic peptides in the company of the USF/Moffitt Cancer Center. Mark still has research ties to LSU, and we hope to see him often.

## Matt Balhoff wins Dow Award

The 2002 recipient of the Dow Award for Excellence in Macromolecular Studies is Mr. Matthew Balhoff. Matt, a 3rd-year graduate student in Chemical Engineering, participates in an IGERT team co-led by Professors Karsten Thompson of Chemical Engineering and William H. Daly of Chemistry. With partner Veronica Holmes of Chemistry, they are exploring and modifying flow in porous media. Matt has interned at Schlumberger in Houston. He has excelled in coursework, even including synthetic chemistry. He promptly and impressively passed his general examination, and has filed mini-grants within the IGERT program to develop experiments that will supplement his simulations. Previous winners were Garrett Doucet and Randy Cush of Chemistry. Like Matt, they received a cash award that can be augmented if the student chooses to use it for travel to enhance their career opportunities.

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## Research Vignette

### Parameter Estimation and Online Modeling of EPDM Process

ExxonMobil Chemical has supported the PhD research of Rujun Li (Drs. Corripio and Dooley, advisors) for the past 4 years. Mr. Li has constructed simulation models of EPDM polymerization and studied applications of various online optimization/control strategies to improve plant productivity and polymer quality. This work has included critical analysis of several mechanisms, including those incorporating long-chain branching and crosslinking. For optimization, a parameter selection technique was developed. By applying novel numerical solution techniques, Mr. Li has accurately modeled the molecular weight distributions of such complex terpolymers both in the pre-gel and post-gel regions. Some of his work appears in:

"Selection of model parameters for off-line parameter estimation", IEEE Transactions on Control Systems Technology, in press

"Dynamic modeling of cross-linking and gelation in continuous ethylene-propylene-diene polymerization reactors using the pseudo-kinetic constant approach.", Chemical Engineering Science, submitted.

Contact Kerry Dooley at [dooley@lsu.edu](mailto:dooley@lsu.edu) if interested in further details on the papers.

## Teaching Vignette

LSU has always nurtured innovative chemical sciences, just look at its leading role in macromolecular chemistry and education! And LSU has done it again. Last spring, Professor David Spivak introduced a cutting-edge new course for LSU: "An Interdisciplinary Introduction to Nanoscience." Nanoscience lecture and laboratory courses provided a highly interdisciplinary environment involving graduate students, undergraduate students, and faculty from Chemistry, Biology, Engineering departments, and CAMD. The IGERT program played a role in sponsoring the visit of Dean Campbell from Bradley University. Through a lecture full of demonstrations using LEGO's, Dean taught the class about nanophase structures of solids, difficult concepts such as magnetoresistance, and how nano-analytical devices work, such as the scanning probe microscope shown in the picture. In addition to nanoscience and macromolecular chemistry, Dr. Spivak

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Matt Balhoff (center) with LSU Alumni and Dow employees Drew Poche' and Alan Chan.

## Thank You

We are grateful to all those who donated to the program last year. Dow continues to be our largest supporter, providing research funds, challenging problems and personnel to assist with student training, seminars and program evaluation. New-comer Islet Technology of St. Paul, Minnesota, has contributed to our unrestricted research program. We enjoy learning about their impressive life science technologies.

LSU Alumnus Dr. Ajit Pendse and friend of the program Dr. Ed Smith continue to assist education by arranging plant tours of ExxonMobil's impressive processing training facility, followed by a tour of the polyethylene plant. As promised in the previous newsletter, we got a photo this time. The green suits and red hardhats matched the Christmas spirit of the visit.



We challenge all our corporate partners to contribute what they can. MSG is an excellent investment in the future. Don't forget about tax-deductible individual contributions to the Macromolecular Development Fund! Many companies will match your individual donation.

## Selected Recent Seminars



Seminar Speaker Paul Dubin with Dave Spivak, Bill Daly and Bob Hammer having lunch at LSU's French House Bistrro. February 13, 2003

For a complete list of future and past seminars, see: <http://macro.lsu.edu/msg/SeminarStuff/seminars.asp>

- David Norwood, Southeastern Louisiana University, *Three Detectors and a Column*
- Lon Mathias, University of Southern Mississippi, University of Southern Mississippi, *Semi-synthetic Polymers Based on Natural Monomers: Biomaterials from Amino Acids.*
- Paul Dubin, Indiana University Purdue University Indianapolis, *Polyelectrolyte Coacervates - Old Package, New Science*
- Tom Seery, University of Connecticut, *Nanocomposite Synthesis.*
- Rigoberto Advincula, University of Houston, *Nanostructured Organic and Polymer Materials: From Ultra Thin Film to Nanoparticles.*
- Ken Shea, University of California Irvine, *Polyethylene One Carbon at a Time.*
- Michael Korn, Southwest Texas State University, *Towards Architectural Control in Synthetic Macromolecules.*
- Eric Simanek, Texas A&M University, *Dendrimers Based on Melamine.*
- Maury Balik, North Carolina State University, *Mechanical Alloying of Polymers.*

*IGERT participants and review panel, October 2003*



*IGERT Retreat and Review, October 2002*





## Selected Recent Publications

MSG Publications are now listed on the web; see:

<http://macro.lsu.edu/msg/Publications2002.htm>

Here are a few samples:

**Selection of model parameters for off-line parameter estimation.**

Li, R. and Dooley, K.M., IEEE Transactions on Control Systems Technology, *in press*.

**The structure and function of CP47 and CP43 in photosystem II.**

Bricker, Terry M.; Frankel, Laurie K. Photosynthesis Research (2002), 72(2), 131-146.

**Zippering up 'the crushed fullerene' C<sub>60</sub>H<sub>30</sub>:C<sub>60</sub> by fifteen-fold,**

**consecutive intramolecular H<sub>2</sub> losses.** Gomez-Lor Berta; Koper Carola; Fokkens Roel H; Vlietstra Edward J; Cleij Thomas J; Jennekens Leonardus W; Nibbering Nico M M; Echavarren Antonio M. Chem. Commun. (Camb) (2002 Feb 21), (4), 370-1.

**Development of high quality poly( $\alpha$ -methylstyrene) mandrels for NIF.**

Takagi, Masaru; Cook, Robert; McQuillan, Barry; Elsner, Fred; Stephens, Richard; Nikroo, Abbas; Gibson, Jane; Paguio, Sally. Fusion Science and Technology (2002), 41(3, Pt. 1), 278-285.

**Sterically Hindered  $\alpha,\alpha$ -Disubstituted  $\alpha$ -Amino Acids: Synthesis**

**from  $\alpha$ -Nitroacetate and Incorporation into Peptides.** Fu, Yanwen; Hammarstroem, Lars G. J.; Miller, Tod J.; Fronczek, Frank R.; McLaughlin, Mark L.; Hammer, Robert P. Journal of Organic Chemistry (2001), 66(21), 7118-7124.

**Cu(0) nanoclusters derived from poly(propylene imine) dendrimer complexes of Cu(II).**

Floriano P N; Noble C O 4th; Schoonmaker J M; Poliakoff E D; McCarley R L Journal of the American Chemical Society (2001 Oct 31), 123(43), 10545-53.

**Amorphous hydrocarbon based thin films for high-aspect-ratio MEMS applications.**

Cao, D. M.; Wang, T.; Feng, B.; Meng, W. J.; Kelly, K. W. Thin Solid Films (2001), 398-399 553-559.

**The influence of maleation on polymer adsorption and fixation, wood surface wettability, and interfacial bonding strength in wood-PVC composites.**

Lu, John Z.; Wu, Qinglin; Negulescu, Ioan I. Wood and Fiber Science (2002), 34(3), 434-459.

**Dynamic modeling of curing process of epoxy prepreg.**

Sun, Liangfeng; Pang, Su-Seng; Sterling, Arthur M.; Negulescu, Ioan I.; Stubblefield, Michael A. Journal of Applied Polymer Science (2002), 86(8), 1911-1923.

**Synthesis of Paucidisperse Poly( $\gamma$ -benzyl- $\alpha$ ,L-glutamate) Oligomers and Star Polymers with Rigid Arms.**

Wang, Xiaolan; Daly, William H.; Russo, Paul; Ngu-Schwemlein, Maria. Biomacromolecules (2001), 2(4), 1214-1219.

**Self-Diffusion of a Rodlike Virus in the Isotropic Phase.**

Cush, Randall C.; Russo, Paul S. Macromolecules (2002), 35(23), 8659-8662.

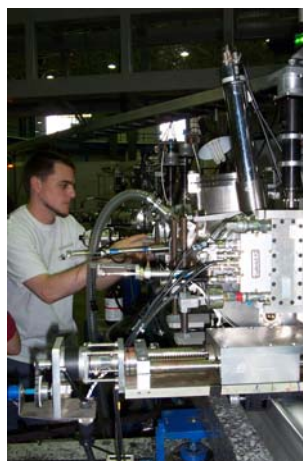
**Systematic study of steric and spatial contributions to molecular recognition by non-covalent imprinted polymers.**

Spivak D A; Campbell J. ANALYST (2001 Jun), 126(6), 793-7.

LSU Faculty and Students have been real globetrotters this year.



LSU students Allison Joubert, Greg Thompson and Professor Vince Licata join Stanford's Ana Gonzales for dinner in Campinas, Brazil, at the Interamerican Workshop on Synchrotron Radiation., December 2002.



Brazil trips are not ALL goofing off. LSU student Jason Campbell worked almost round the clock on the beautiful Brazilian SAXS line. May, 2002.

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## Selected Recent Publications, continued.

**Chromophore formation in resorcinarene solutions and the visual detection of mono- and oligosaccharides.** He, Ming; Johnson, Rolanda J.; Escobedo, Jorge O.; Beck, Patricia A.; Kim, Kyu Kwang; St. Luce, Nadia N.; Davis, Claude J.; Lewis, Patrick T.; Fronczek, Frank R.; Melancon, Bruce J.; Mrse, Anthony A.; Treleaven, W. Dale; Strongin, Robert M.. *Journal of the American Chemical Society* (2002), 124(18), 5000-5009.

**Denucleation Rates during Ostwald Ripening: Distribution Kinetics of Unstable Clusters.** Madras, G.; McCoy, B.J. *Journal of Chemical Physics* (2002) 117:6607-6614.

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## Alliances

LSU is building alliances with sister universities in Louisiana. Governor Foster's Vision 2020 program lists Materials Science as an area for targeted growth. Polymers and biopolymers will surely be a part. Subsequent to a workshop sponsored by the Louisiana Board of Regents, an inventory of Louisiana's macromolecular capabilities was conducted. It is impressive! If it involves polymers, it can almost surely be done in Louisiana. Few if any states have more to offer. The three largest academic programs—at Tulane University, University of Louisiana Lafayette and LSU—have agreed to coordinate a statewide effort to build on these strengths. The program will be designed to enhance service to regional industry, help attract new businesses to our state, ensure a steady flow of great students and faculty, and improve the quality of research ideas and infrastructure.

If you or your company might be interested in this, please let us know (by e-mail: paul.russo@chem.LSU.edu or 225-578-5729). Your interest will be channeled to the most appropriate Louisiana resource. At Tulane, the polymer effort is organized around the Tulane Institute for Macromolecular Engineering and Science. TIMES is the recent recipient of a large NASA appropriation; their progress is remarkable. At the University of Louisiana Lafayette, the coordinating body is the Manufacturing Extension Partnership of Louisiana (MEPoL) which targets improved business practice and efficiency.

# TIMES

[Tulane Institute for Macromolecular Engineering and Science](http://www.tulane.edu/~times/)

<http://www.tulane.edu/~times/>



[MEPoL Manufacturing Extension Partnership of Louisiana](http://www.mepol.org/index.html)

<http://www.mepol.org/index.html>



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