PTC
POLYMER TECHNOLOGY CENTER
TEXAS A&M ENGINEERING EXPERIMENT STATION

Fourth Quarter 2013

NEWSLETTER

Mark Your Calendars for PTC'S upcoming events:

* SCRATCH Consortium = October 24th, 2013 Texas A&M University, College Station, TX
* PTIC Consortium = October 24th-25th, 2013 Texas A&M University, College Station, TX
* APPEAL Consortium = November 15th, 2013 2121 W. Holcombe Blvd., Houston, TX

Inside the Newsletter...

Kaneka Americas Holding, INC. (KAH) Scholarship Fund

Kaneka Americas Holding, Inc., a member of the SCRATCH Behavior of Polymers Consortium with the Polymer Technology Center at Texas A&M University, has generously funded a scholarship supporting junior faculty, visiting scholars, and students involved in materials science-related research and academics at Texas A&M University. Initial funding period of scholarship funding, 2014 through 2016, in the amount of $20,000 per year, with the possibility for extension. Eligible graduate students are those conducting research in material science or organic chemistry fields. Eligible undergraduate students must be enrolled in at least one material science and engineering course. PTC would like to express its gratitude to Kaneka Americas Holding, Inc., for its generosity to the junior faculty, visiting scholar and student support at Texas A&M University. For more information regarding this scholarship, please periodically visit the PTC website at: http://ptc.tamu.edu/.

Newest APPEAL member

PTC is pleased to announce and welcome our newest Voting APPEAL Consortium member, Element.

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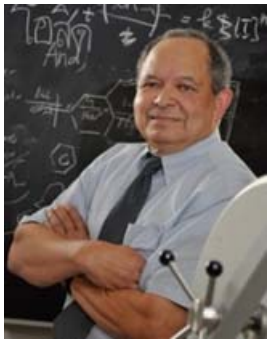
TEXAS A&M UNIVERSITY

The CO_2-Epoxide Copolymerization: Computational-Experimental Synergy

Andrew D. Yeung,[1]
Donald J. Darensbourg,
Department of Chemistry



Copolymerization of carbon dioxide with epoxides yields polycarbonates with useful physical properties and converts undesired CO_2 into valuable feedstock. We have recently begun using computations to supplement our existing experimental work.

To set the stage, we developed a reliable method for studying the thermodynamics of the copolymerization.[2] Performed early on, these calculations help us avoid attempting reactions that are unequivocally unfavorable on thermodynamic grounds.

Feedback between computations and experiments accelerates our research, exemplified by our recent study on poly(cyclopentene carbonate) degradation. Experimentally, the polymer was found to degrade to cyclopentene oxide, instead of trans-cyclopentene carbonate. Calculations quickly confirmed that the former product was favored (Fig. 1). These also suggested that CO_2 removal would enhance the degradation, borne out by subsequent experiments. In this manner, we devised a way to efficiently recycle poly(cyclopentene carbonate) to the co-monomers, to be recycled into polymers with uncompromised physical properties.[3,4]

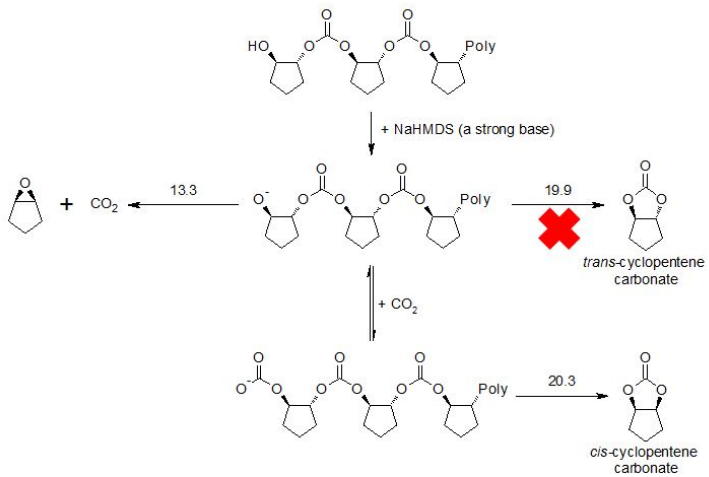


Fig. 1. Computations fully explain poly(cyclopentene carbonate)'s degradation. The alkoxide degrades to the co-monomers, the carbonate degrades to the *cis*-cyclic carbonate, and the thermodynamically-unstable *trans*-cyclopentene carbonate with two *trans*-fused five-membered rings is not observed. (ΔG‡ noted, kcal/mol)

Our recent foray into computational chemistry has provided our group with greater insight into the CO_2-epoxide copolymerization. More importantly, synergy due to computational-experimental collaboration has brought our group success.

Kevin White, Graduate Assistant Research

Kevin White, a member of Professor H.-J. Sue's research group, successfully defended his Ph.D. dissertation this fall and will receive his doctorate in Mechanical Engineering in December. Kevin began to work with Professor Sue's research group in Spring 2008 as an undergraduate student worker and has since made significant contributions to several projects in the group, including work on carbon nanotube composites in epoxy and polypropylene systems, multi-scale carbon fiber reinforced composites, and properties of high-pressure, high-temperature thermoplastics. His dissertation research has focused on the rheology of model nanoparticles dispersed in an epoxy monomer. The research focused on suspensions of model nanoparticles with high aspect ratio and well-defined geometry. The primary nanoparticles of interest were carbon nanotubes and α-zirconium phosphate nanoplatelets. Hybrid systems containing both nanoparticles, which interact through electrostatic tethering, were also investigated. Kevin's ongoing research interests are centered around practical and efficient development of advanced materials by understanding the fundamental mechanisms involved in reinforcement.

Dr. Lin Jin, PTC PostDoc

Howdy.

This is Lin Jin. I have been working as a Postdoc researcher at the Polymer Technology Center (PTC) for about two years. My research experience at Texas A&M University was mainly about residual stress analysis and morphology characterizations of PAEK materials. I learned and enjoyed a lot during this period of time.

I would like to thank Dr. Sue and Dr. Bremner for giving me this opportunity to work in the excellent research environment, and I appreciate all the help and support from our group.

Thank you,

Lin Jin

Footnotes for Dr. Darensbourg article

1. Andrew D. Yeung obtained his B.Sc. (Hons) from the National University of Singapore. He is currently a fourth year Ph.D. candidate in Chemistry in the Darensbourg Research Group.

2. Darensbourg, D. J.; Yeung, A. D. *Macromolecules* 2013, *46*, 83.
3. Darensbourg, D. J.; Yeung, A. D.; Wei, S.-H. *Green Chem.* 2013, *15*, 1578.
4. Darensbourg, D. J.; Wei, S.-H.; Yeung, A. D.; Ellis, W. C. *Macromolecules* 2013, *46*, 5850.

Loftin Announces Plans For The Future

On July 12, 2013, Dr. R. Bowen Loftin announced that he will step down as president of Texas A&M University effective January 13, 2014.

With his resignation, Dr. Loftin will be returning to the faculty and will serve as a tenured professor in the Department of Industrial and Systems Engineering in the Dwight Look College of Engineering. The university also plans to assist Loftin in establishing an institute that will focus on advanced, state-of-the-art modeling and simulation in human behavioral modeling in terrorist organizations and the spread of diseases among human and animal populations.

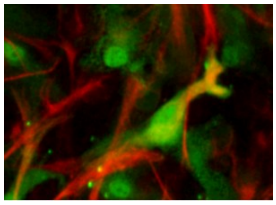
Full Story: http://tamutimes.tamu.edu/2013/07/12/loftin-announces-plans-for-the-future/

Texas A&M Among Top Three Universities In Rankings That Emphasize Service To The Nation

Texas A&M is rated as one of the top three universities in the nation in the 2013 poll announced August 27, 2013 by *Washington Monthly*, which puts special emphasis on service to the nation.

Full Story: http://tamutimes.tamu.edu/2013/08/27/texas-am-among-top-three-universities-in-rankings-that-emphasize-service-to-the-nation/

Researchers Finding New Clues To Beat MS

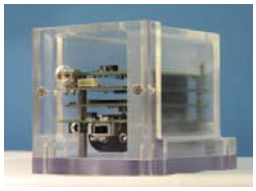


Astrocytes (red) were treated with tumor necrosis factor in culture and the expression of galectin-9 examined (green). Astrocytes expressing galectin-9 are shown in yellow. Photo: Texas A&M University

Multiple sclerosis (MS) is a disease that affects the central nervous system (the brain and spinal cord) with devastating consequences. The cause of MS is still unknown, but it is clear that the disease is perpetuated by repeated attacks of the nervous system by cells from a person's own immune system. Texas A&M University researchers in the College of Veterinary Medicine & Biomedical Sciences and the Texas A&M Institute for Neuroscience have uncovered a pathway that the brain cells use to blunt these attacking immune cells.

Full Story: http://tamutimes.tamu.edu/2013/08/15/researchers-finding-new-clues-to-beat-ms/?utm_source=tamutimes&utm_medium=email&utm_campaign=2013-08-20

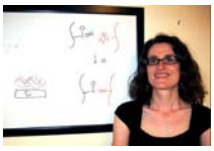
Texas A&M engineering students to collaborate with NASA



Engineers from NASA's Johnson Space Center will be collaborating with students in the Electronic Systems Engineering Technology (ESET) Program at Texas A&M University to develop space-qualified hardware systems. NASA is looking to expand the capabilities of its Modular Integrated Stackable Layer (MISL) platform, while Texas A&M students and faculty will gain valuable experience working with state-of-the-art technologies.

Full Story: http://engineering.tamu.edu/news/2013/08/23/texas-am-engineering-students-to-collaborate-with-nasa?utm_source=tamutimes&utm_medium=email&utm_campaign=2013-08-27

Lutkenhaus named ACS PMSE Young Investigator



Dr. Jodie Lutkenhaus is one of 13 Young Investigators chosen to present next spring. The presenters were chosen from academia, government, and industry. All researchers are within seven years of having completed their graduate or postdoctoral studies and have made significant contributions to their respective fields in that time.

Full story: http://engineering.tamu.edu/news/2013/07/15/jodie-lutkenhaus-is-named-a-2014-acs-pmse-young-investigator

Dr. Mustafa Akbulut receives DARPA Young Faculty Award 2013

Akbulut received the DARPA Young Faculty Award for his proposal, Next-Generation Soldiers Involving Dispersion of Soft Ligand Functionalized Boron Nitride Nanoribbons or Nanosheets in Alloys as Thermal Interface Materials (TIMs).

Full story: http://engineering.tamu.edu/news/2013/08/30/akbulut-receives-darpa-young-faculty-award-2013

Dr. Wayne Nguyen P. Hung appointed Charlotte and Walter Buchanan Faculty Fellow

Dr. M. Katherine Banks, vice chancellor and dean of engineering, has appointed Dr. Wayne Hung the Charlotte and Walter Buchanan Faculty Fellow in Engineering Technology.

Full story: http://engineering.tamu.edu/news/2013/08/30/hung-appointed-charlotte-and-walter-buchanan-faculty-fellow

Chemical engineering professor awarded NASA grant

Dr. Zhengdong Cheng, associate professor in the Artie McFerrin Department of Chemical Engineering at Texas A&M University, was awarded a grant from NASA for his research in nanoplate technology.

Full Story: http://engineering.tamu.edu/news/2013/08/22/chemical-engineering-professor-awarded-nasa-grant

Grunlan elected PMSE secretary

Dr. Melissa Grunlan, associate professor in the Department of Biomedical Engineering at Texas A&M University, has been elected secretary of Polymeric Materials: Science and Engineering (PMSE), a division of the American Chemical Society.

Full Story: http://engineering.tamu.edu/news/2013/09/23/grunlan-pmse

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TAMU/SPE Student Chapter Upcoming Activities
BY Adriana Pavia

Howdy Ags!

Although the semester is still young, the society of plastics engineers is already off to a great start! I want to thank all of our active members and everyone else who has participated and contributed to this.

We started off our semester last month with a seminar talk by Dow Fellow, Dr. Ravindra Dixit, in which he shared some of his experiences at Dow, with special attention to the control of polymer properties through innovations in catalysts and processes.

In October, we will have the pleasure of hosting Michael Mullins, the executive associate dean and director of the laboratory for molecular simulation; his talk will be very different from our usual seminar talks, as he will be discussing a side of research and development that few of us ever think about: the ethical aspect of research.

For our November and December seminars, we will be hosting two non-traditional speakers from small commercial companies, MECX and Chemical Data.

We also have several community outreach activities planned for this semester, including the Chemistry Open House and Expanding Your Horizons in October and December, respectively.

TBA: We are still working on scheduling our semester plant tour. However, our plant tour for May 2014 has been finalized for the South Texas Project Nuclear Operating Company.

Monthly seminars, as always, are open to everyone, but if you are interested in taking part in our plant tours or other events, you will need to become a national SPE Member. If you are interested, please email me at adriana.pavia@chem.tamu.edu for an application. The fee is $31 for student members, but we will subsidize part of the cost for you to bring the price down to $25.

If you have any questions or suggestions, do not hesitate to contact us at plastics@plastics.tamu.edu. Also, be sure to visit our website, **http://plastics.tamu.edu**, for chapter news, seminar information, events, membership information, research highlights, and chapter photos.

Thanks and gig 'em,
Adriana Pavia-Sanders, SPE President, TAMU Student Chapter

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For more information: http://ptc.tamu.edu/certificate.html	

TAMU/SPE Student Chapter

To find out more about the TAMU/SPE Student Chapter, please contact Adriana Pavia at:
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Visit the SPE Student Chapter website at:
http://plastics.tamu.edu

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Edited by: Ayotomiwa Babalola & Megan Nicholson

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Q-4 2013