

The HOWARD P. ISERMANN DEPARTMENT OF CHEMICAL AND BIOLOGICAL ENGINEERING

# **CBE Seminar Series – Fall 2020**

## Dr. Carlos R López-Barrón

Staff Scientist ExxonMobil

### Seminar: Wednesday, October 7, 2020 12:00 p.m. (ONLINE)

WebEx link:

https://rensselaer.webex.com/rensselaer/onstage/g.php?MTID=e8bf7f97b7c60e14bce6e2ac3254dd125 Password: CBESeminar

## "Bottlebrush Polyolefin Elastomers"

#### Abstract:

The extreme conformation of molecular bottlebrushes (i.e., very rigid backbones and high graft density) provides unique rheological and mechanical properties to these class of polymers, compared to the linear counterparts. One of such properties is the very low elastic modulus (resulting from very large entanglement molecular weight); a property that has could be used to produce super-soft elastomers [Polymer 47, 7198 (2006)] via crosslinking. A number of multi-step chemical paths have been reported in the literature to produce the required functionalities for bottlebrush molecules to undergo physical or chemical crosslinking reactions. However, form a practical standpoint, it is highly desirable to produce elastomers in a single step and using available commercial catalyst systems. We synthesized a series of ultra-high molecular weight (UHMW)  $poly(\alpha$ -olefin) (P $\alpha$ O) molecular bottlebrushes by organometallic coordinative insertion polymerization of 1-alkenes with lengths ranging from 10 to 18 carbons. It was recently reported that these Pao bottlebrushes crystallize exclusively by side chain crystallization [Macromolecules 51, 17, 6958 (2018)]. Interestingly, they show two thermal transitions under heating. Combining DSC, rheology, microscopy and X-ray scattering measurements, we were able to determine that the first transition is an order-order transition (OOT) from a brittle and highly crystalline plastic to a soft and elastic solid with lower crystallinity. The second transition is the complete melting of the remaining crystals. To our knowledge, this is the first report of an OOT in a homopolymer. The most remarkable observation is that at the intermediate temperature, above the OOT and below melting, these P $\alpha$ O bottlebrushes behave as soft elastomers with extremely large extensibility (strain to break > 3000%) and significant elastic recovery (tensile set ~40%). Both the OOT and melting transitions are entirely reversible. Hence, these materials are the first reported thermoplastic elastomers (TPE), for which the origin of the elastomeric properties is side-chain crystallization. Lastly, I will discuss the origins of the elastomeric behavior in the Pao bottlebrushes, which we investigated using a combination of in-situ time-resolved SAXS/WAXS, SANS and SALS measurements.

#### **Biography:**

Dr. López-Barrón received a Bachelor's degree in Chemical Engineering from the Universidad Nacional Autonoma de Mexico (UNAM) in 1998 and a Master degree from Universidad de Guadalajara (Mexico) in 2002. In 2009, he received a PhD degree in Chemical Engineering from the University of Minnesota. He accepted a post-doctoral assignment at the Center for Neutron Science of the University of Delaware from 2009 to 2011, where he conducted fundamental research on the relation between the rheology and structure of soft materials using neutron scattering techniques. He joined ExxonMobil Chemical in Baytown, Texas as a staff scientist in 2011, and currently holds several technical assignments including fundamental and applied work in polyolefins and their blends, polyolefin-based elastomers.

Due to COVID-19, no refreshments will be available for this seminar.

For more information, please contact Lisa Martin (swishl@rpi.edu) or Helen Zha (zhar@rpi.edu)