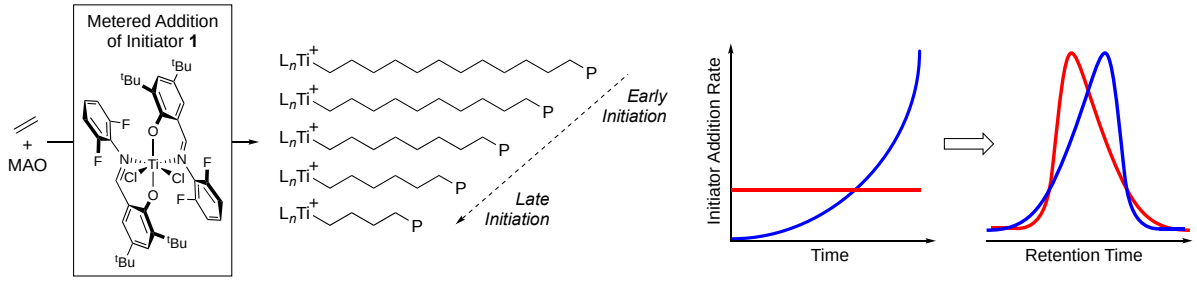
Controlling the Shape of Molecular Weight Distributions in Coordination Polymerization and Its Impact on Physical Properties *(March 2020)*

Innovation through synergy
Centers for Chemical Innovation

The NSF Center for Sustainable Polymers (CSP) connects scientists from the University of Minnesota, Cornell University, Northwestern University, the University of California, Berkeley, Washington University in St. Louis, the University of Chicago, and the University of South Dakota in a manner that promotes highly collaborative research. This environment allows partnership across various scientific disciplines, including polymer, organic, biological, inorganic, and theoretical chemistry. As such, CSP researchers have been able to approach challenging problems related to sustainability with a wide range of expertise.

High-density polyethylene (HDPE) is a semicrystalline thermoplastic that can be processed into a versatile range of commodity materials such as storage containers, plastic bags, pipes, electrical coatings, and much more. Due to its chemical resistance, high tensile strength, and light weight, HDPE is a prominent commodity plastic with over 50 million metric tons produced annually at a value of 63 billion US dollars. Thus, development of new methods to control the properties and processability of HDPE is vital for reducing the energy costs of polyolefin processing and minimizing the quantity of plastic used in commercial grade materials.



Metered addition of a titanium phenoxyimine initiator allows for MWD shape control of HDPE which in turn leads to lower viscosity without compromise of tensile strength.

Previous studies have shown that variations in polymer dispersity (*Đ*) and polymer blending influence the properties of HDPE. However, little work has been done to understand how the shape of the molecular weight distribution (MWD) influences polymer properties. To address the CSP's grand challenge of developing high performance sustainable plastics, a team of researchers from Cornell comprising of Omar Padilla-Vélez, Renee Sifri, Brett Fors, and Geoff Coates investigated the effects of MWD shape on the properties and processability of HDPE. By adding a titanium phenoxyimine initiator at different rates and times into a solution of ethylene, the MWD shape of HDPE can be controlled. Rheological and tensile testing of these samples revealed that MWD shape had a profound influence on complex viscosity but did not impact tensile strength; leading to future promise in lowering processing energies of HDPE production without compromising material properties. This collaboration benefited from the use of synthetic methods to control MWD shape of living polymerizations (Fors) and the expertise of living catalysts for polyolefin synthesis (Coates). Further studies will be done to mathematically model how higher moments of a polymer's distribution function influence the physical properties of polyolefins in collaboration with Rob Distasio at Cornell.

Sifri, R. J.; Padilla-Vélez, O.; Coates, G.W.; Fors, B.P Controlling the Shape of Molecular Weight Distributions in Coordination Polymerization and Its Impact on Physical Properties. *J. Am. Chem. Soc.*, **2020**, 142, 1443-1448.