Machine Learning Guided Discovery of Stereoselective Polymerization Catalysts

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Poly(lactic acid) (PLA) is a leading biodegradable and biocompatible polymer with growing importance in the plastics industry. Stereoselective ring-opening polymerization of lactide provides access to stereoregular PLA with thermal and mechanical properties superior to those of atactic PLA. However, the discovery of highly stereoselective polymerization catalysts remains largely empirical, relying on extensive synthesis and experimental screening. To address this challenge, we developed an integrated computational–experimental framework for efficient and predictive catalyst discovery and optimization. We first established a Bayesian optimization workflow using a subset of literature data on stereoselective lactide ring-opening polymerization. Guided by this algorithm, we identified multiple new aluminum complexes exhibiting either isoselective or heteroselective polymerization behavior. We recently expanded this framework by incorporating in-loop analysis and global–local molecular descriptors, enabling the discovery of highly efficient enantioselective catalysts to produce stereocomplex PLA, which exhibits enhanced thermal and mechanical properties compared to other PLA stereoisomers.

Brief CV:

Dr. Rong Tong received his Ph.D. degree in Materials Science and Engineering from the University of Illinois at Urbana-Champaign in 2010, working on the synthesis and formulation of novel nanomedicines for targeted cancer therapy. He was a postdoctoral associate at both Massachusetts Institute of Technology (Langer lab) and Harvard Medical School (Kohane lab) during 2010 to 2015. He is currently an Associate Professor in the Department of Chemical Engineering at Virginia Tech. His research interests include polymer chemistry, biomaterials and targeted cancer therapy. He is the recipient of Thieme Chemistry Journals Award (2020), Class of Influential Researcher of Industrial & Engineering Chemistry Research (2017), Emerging Investigator of Biomaterials Science (2017), American Chemical Society AkzoNobel Award in polymer chemistry (2010), Racheff-Intel Graduate Student Research Award (2009), the Siteman Center for Cancer Nanotechnology Fellowship (2007).