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POLYMER MACROCYCLES: A NOVEL TOPOLOGY TO CONTROL DYNAMICS OF RUBBERY MATERIALS



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Understanding the dynamics of polymers of different topologies is an important field of study and one of the most important unanswered questions in this field is "how do circular polymers" move in the melt state. Furthermore, there is new information that also suggests that molecular topology, specifically circular rings, impacts the response of materials in nanometer-scale confinement. The proposed work addresses these subjects through a collaboration in which specialists in polymer synthesis, polymer rheology and scattering methods, and in the physics of nanoconfinement work together to tackle the problem of the thermophysical behavior of circular macromolecules. A new synthesis method of "green" oxidative polymerization, which produces high purity macrocycles, will be used to produce high purity circular polyisobutylene-based rings for thermophysical characterization including linear rheology from creep and creep recovery and dynamic mechanical testing to fully characterize dynamics to entanglement densities higher than previously obtainable with synthetic polymers. Critical edge fractionation and direct visualization of the circular polymers and any linear contamination through the use of polymer amplification methods combined with atomic force microscopy will directly image the numbers of circular and linear molecules in each sample. The complementary expertise of the groups will provide breakthrough knowledge and understanding of the dynamics of macrocyclic polymers as well as the response of these novel materials to nanoconfinement effects. The strong differences in behavior between linear chains and the circular macromolecules also provides an important opportunity to break the "magic triangle" of tire technology that relates, in particular, to rolling resistance and consequent fuel consumption. For the first time, it becomes a potentiality to be able to reduce the magnitude of the so-called Payne effect in reinforced rubbers because circular macromolecules have reduced nanoconfinement sensitivity relative to their linear counterparts. The application of a novel "green" chemistry that can create high purity, high molecular weight circular macromolecules is an important tool to complete our understanding of the dynamics of circular polymers. Here we have identified and propose to resolve several important areas: 1) a need for high-molar mass rings with high purity; 2) purification and verification of rings, 3) slow modes and scaling of viscosity with molar mass; 4) non-linear rheology; 5) impact of circular topology on the glass transition behavior at the nanoscale and nano-mechanical response in freely standing films; 6) Impact of circular topology on the Payne effect in filler reinforced rubber. The proposal addresses these challenges by synthesizing pure rings and providing the molecules to the team for rheological characterization and testing and for nano-mechanical and nano-calorimetric methods. The potential outcome is to resolve important issues in polymer dynamics that are related to the unique topology of the ring architecture. The proposed work develops novel synthetic capabilities and combines them with excellent physical and rheological characterization techniques to move the field forward in a dramatic fashion. Theories will be tested, and experiments will be moved into domains not previously achievable with synthetic polymers. The work promises to open new frontiers in elastomers, especially in tire technology by potentially altering the magic triangle of rolling resistance, traction and wear due to reduced Payne effects in reinforced systems.