STEP-GROWTH POLYMERS AS MACRO CHAIN TRANSFER AGENTS – AN EXPERIMENTAL AND THEORETICAL STUDY

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ABSTRACT

In this contribution, we present a unique combination of step-growth and chain-growth polymerization, where a fast and highly efficient photo-induced step-growth polymerization generates macro-RAFT species, consisting of a designed trithiocarbonate chain transfer agent and a photoactive ortho-methyl benzylaldehyde compound. The generated macro-RAFT species enables a subsequent chain extension via RAFT polymerization within the polymer chain with species up to 20 kg/mol, equal to a total of 20 repeating units. For the RAFT polymerization styrene was employed as monomer, achieving species with molecular weights after the chain extension of 1000 kg/mol. The unique combination of two intertwined polymerization mechanisms is highly complex in nature, since the step-growth macro-RAFT polymer offers various possibilities to insert a monomer unit during the RAFT polymerization. Therefore, we simulated the subsequent RAFT process in a full kinetic reaction scheme. Specifically, stochastic modeling tools are applied to allow for a detailed kinetic analysis of the polymerization. The complete reaction event history of the individual chains is tracked, enabling a mapping of the evolution of RAFT groups and styrene insertions into the chains in this complex reaction system. Although the insertion of the monomer units within the growing chain and the fragmentation during the RAFT mechanism represent statistical processes, we achieved good agreement of theoretical calculations and experimental findings.

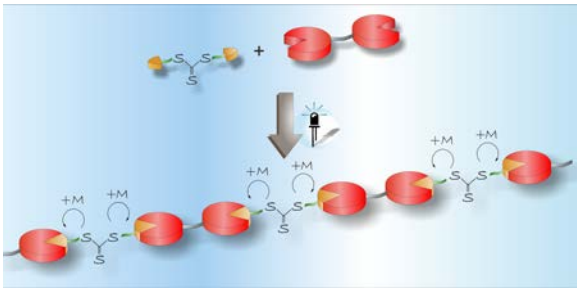

Figure 1. Light-induced step-growth polymerization with subsequent chain extension *via* RAFT polymerization.

References:

Gegenhuber, T; De Keer, L.; Goldmann, A. S.; D´hooge, D. R.; Barner-Kowollik, C. **2016**, submitted.