In silico based design of nitroxide mediated polymerization: from homopolymers to sequence controlled polymers

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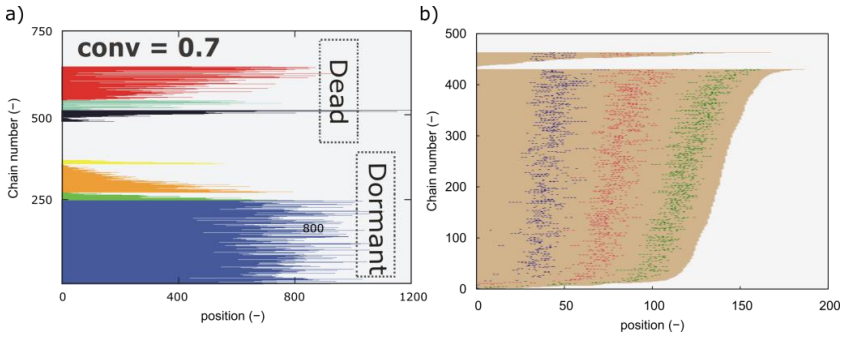
Abstract

Model-based design is applied for nitroxide mediated polymerization (NMP; [1, 2]), considering both homopolymers and sequence controlled polymers, as obtained via nitroxide mediated copolymerization of an electron-donor monomer with discrete additions of an electron-acceptor monomer (*e.g.* an *n*-substituted maleimide) [3]. Improved NMP specific Arrhenius parameters are first reported for styrene homopolymerization with BlocBuilder MA, based on regression to an extensive set of experimental data. Using matrix-based kinetic Monte Carlo simulations a visualization of individual chains is performed. This allows to explicitly differentiate between polymer chains according to their living nature, and chain initiation and dead polymer formation mechanism for the dormant and dead polymer chains, respectively (Figure 1a) [4]. Multi-objective optimization of the NMP of styrene is subsequently performed, clearly indicating the beneficial use of temperature- and fed-batch monomer programs [5]. Finally, novel insights and optimization pathways for sequence controlled polymers are provided, including the explicit visualization of the position of the functional monomer units for each individual chain (Figure 1b).



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