A generic platform for the visualization of all monomer sequences in individual copolymer chains

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INTRODUCTION
One of the key challenges for future polymer synthesis is the detailed characterization of individual macromolecules, including the position of all monomer units and functional groups. In this contribution, we demonstrate that advanced modeling techniques in combination with detailed experimental procedures allow to overcome this challenge. These techniques are further used to identify the most suitable protocols for the synthesis of advanced macromolecular architectures, accounting for the possible impact of diffusional limitations and side reactions. Examples are included both for radical and cationic processes. The presented modeling platform is generic and can lead to a significant progress in the field of macromolecular engineering.

NITROXIDE MEDIATED POLYMERIZATION

Estimation of NMP specific Arrhenius parameters

Insight into side reactions during NMP of styrene

Chain extension with n-butyl acrylate:

→ 110°C to ensure increased end group functionality, while 130°C ensure low reaction time

CATIONIC RING OPENING POLYMERIZATION

TCL = 100

with chain transfer (real)
X_m = 0.25 X_m = 0.50

without chain transfer (idealized)
X_m = 1.0

SEQUENCE-CONTROLLED COPOLYMERS

• Combination of e-donor and e-acceptor monomers
• In silico synthesis of a trifunctional copolymer

Macromolecular design via the interchange of xanthates

→ 1 exchange cycle per dormant chain
→ estimation of C_m(x)

CONCLUSIONS

• A generic platform is developed for polymer design accounting for side reactions and diffusional limitations
• Visualization of all monomer sequences is possible using a kinetic Monte Carlo algorithm, recording every reaction event an individual growing polymer molecule undergoes
• Insight into the mechanisms behind chain-to-chain deviations
• Experimental validation whenever possible, combined with model-based design via selection of agents and reaction conditions

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