ABSTRACT SYMPOSIUM NAME: 3rd Symposium on Poly(2-Oxazoline)s & Polypeptoids-Oral

ABSTRACT SYMPOSIUM PROGRAM AREA NAME: POLY

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TITLE: Model-based design of the microstructure of individual copoly(2-oxaziline) chains

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ABSTRACT BODY:

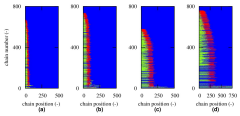
Abstract: To enhance to understanding of copolymerization kinetics and the impact of the synthesis conditions on the polymer microstructure advanced modeling techniques such as kinetic Monte Carlo (*k*MC) simulations are a powerful tool.[1,2,3] In the present contribution, the potential of *k*MC simulations to design the comonomer incorporation in the synthesis of well-defined copoly(2-oxazolines) via cationic ring-opening polymerization (CROP) is illustrated. Based on a comparison with an extensive set of polymerization data, the model parameters are optimized.[4] Both the synthesis of steep gradient copolymers and copolymers with precision control on side-group functionality are considered. It is specifically highlighted that modeling allows to visualize all the comonomer sequences for each individual chain (see figure; target degree of polymerization (target DP): 50, 100, 200, and 400), offering a strong support toward experimental characterization techniques and therefore opening the pathway of the full exploitation of the CROP technique.

[1] P.H.M. Van Steenberge, D. R. D'hooge, Y. Wang, M. Zhong, M.-F. Reyniers, D. Konkolowicz, K. Matyjaszewski, G.B. Marin Macromolecules 2012, 45, 8519.

[2] D.R. D'hooge, P.H.M. Van Steenberge, P. Derboven, M.F. Reyniers, G.B. Marin, Polym. Chem. 2015, 6, 7081.

[3] D.R. D'hooge, P.H.M. Van Steenberge, M.-F. Reyniers, G.B. Marin Prog. Polym. Sci. 2016, provisionally accepted.

[4] P.H.M. Van Steenberge, B. Verbraeken, M.F. Reyniers, R. Hoogenboom, D.R. D'hooge Macromolecules 2015, 48, 7765.



Vizualisation of monomer sequences of individual chains with increasing target DP