# Abstract Preview of 'DD' (J97JQH)

This is a summary of your **2017 67th Canadian Chemical Engineering Conference** webHermes abstract. Once you have verified that it is correct you should print a copy for your records.

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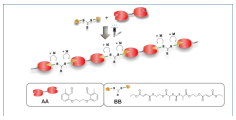
| Prepared by | Dagmar D'hooge *dagmar.dhooge@ugent.be* |
| Preferred Symposium | Macromolecular Sciences and Engineering |
| Preferred Session | New Polymers and Polymerization Techniques |
| Allow Recording | No |
| Invited Speaker | No |
| Preferred Presentation | Oral |
| Poster Competition | No |
| Learning Outcomes | Ideal reaction conditions for a unique combination of step- and chain-growth polymerization |
| Audio/Visual | not applicable |

## Preview of your abstract

**Model-based design of reaction conditions for segmented copolymer synthesis by combining step - and chain-growth polymerization** **L De Keer** *<lies.dekeer@ugent.be>*, **PHM Van Steenberge** *<paul.vansteenberge@ugent.be>*, **MF Reyniers** *<mariefrancoise.reyniers@ugent.be>* and **DR D'hooge**[*$] *<dagmar.dhooge@ugent.be>*, LCT, Ghent University; **T Gegenhuber** *<thomas.gegenhuber@kit.edu>*, **A j**[a,b] *<a.goldmann@qut.edu.au>* and **C. Barner-Kowollik**[a,b] *<christopher.barnerkowollik@qut.edu.au>*, [a]Queensland University of Technology; [b]Karlsruhe Institute of Technology



Model-based design using bivariate kinetic Monte Carlo (kMC) simulations is applied to identify suited reaction conditions to obtain high molar mass segmented copolymers, employing a unique combination of light driven Diels Alder based step-growth and reversible addition fragmentation chain transfer (RAFT) polymerization. For the step-growth precursor polymer synthesis, off-stoichiometric conditions ($r$ = $[AA]_0$: $[BB]_0$ =1.5) need to be used to ensure the optimal compensation for unexpected AA homopolymer formation. The optimal $r$ value is based on a detailed product distribution analysis using a kMC model comprising of over 200 reactions and approximately 20 macrospecies types and taking into account practical constraints such as the reaction time and solubility limits. For the RAFT polymerization, it is demonstrated *in silico* that the optimized conditions at 60°C allow to incorporate well defined polystyrene segments (on average 100 monomer units) in the BB units of the original step-growth polymer and the disturbance of unwanted AA homopolymer segments is very low.

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