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Design of radical polymerization products in homo- and heterogeneous media

Aim

Development of a computer model for the design of recyclable polyolefins and polymer brushes.

Justification

First-principles design of polymeric materials is gaining in importance.

A first example is the emergence of intelligent design of engineering plastics toward easy recycling, namely the incorporation of (bio)degradable ester linkages in polyolefins during their production. The LCT has recently published a combined kinetic modeling and experimental study on such environment-friendly production of futuristic plastic materials. It appears that the segment length of polyolefins between ester linkages must be strictly controlled to guarantee biodegradability. Hence, a next step is to build a computer model for the production in a (semi-batch) reactor to control the segment length of the copoly(ester-olefin)s. This research is expected to also have importance for applications in tissue engineering.

A second example are surface-tethered polymers (see Figure 1). Applications include coatings for anti-fouling and corrosion protection, purification, drug and gene delivery, biosensing, novel adhesive materials for tissue engineering, protein-resistant biosurfaces, chemical lubricants, and polymer carriers for controlled-release of active compounds. The LCT has recently developed an advanced computer model to predict the conformations of surface-tethered polymers (see Figure 1), but it is limited to living polymerization mechanisms for the time being and it also requires benchmarking with a method of moments method.

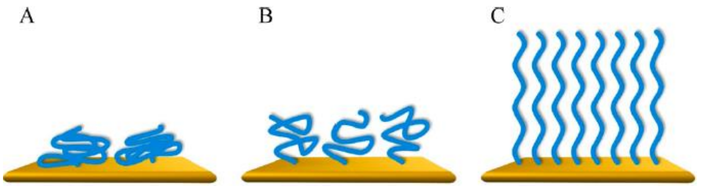

Figure 1: Three regimes of conformations of surface-tethered polymer chains: A) pancake, B) mushroom, C) brush.

Program

1. Literature study on radical polymerization in solution and initiated from a solid surface.
2. Development of a computer model for the production of poly(ester-olefins)s in solution via radical polymerization of cyclic ketene acetals and ethylene in semi-batch reactors and continuous stirred tank reactors.
3. Development of a computational model for brush synthesis via living surface-tethered polymerization toward a RAFT mechanism.
4. Exploration of feasibility to extend an existing kinetic Monte Carlo model for living brush synthesis toward a RAFT mechanism.

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