Supplementary Information

Modular addition strategy-regulated polymerization-induced self-assembly: an *in-silico* experiment

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Table S1. The addition time and the addition amount of initiators in each system and the correspondences between the simulation and a true experiment.

System	macro-CTA addition mode	The *i*-th macro-CTA addition	Addition time point of macro-CTA		Addition amount of macro-CTA	
			Simulation	Experiment	Simulation	Experiment
			$t_{add}(i)$	$t_{add}(i)$	$n_{init}(i)$	$m_{init}(i)$
System of Fig. 2a	Benchmark	1	-	-	3000	0.4725 mmol, (2.47 ml)
		Reaction finished	1×10^7 step	28 h	-	-
	Scenario I	1	0	0	1000	0.1575 mmol, (0.823 mL)
		2	3×10^6 step	8 h	1000	0.1575 mmol, (0.823 mL)
		3	6×10^6 step	16 h	1000	0.1575 mmol, (0.824 mL)
		Reaction finished	1×10^7 step	28 h	-	-
	Scenario II	1	0	0	1000	0.1575 mmol, (0.823 mL)
		2	5×10^6 step	14 h	1000	0.1575 mmol, (0.823 mL)
		3	1×10^7 step	28 h	1000	0.1575 mmol, (0.824 mL)
		Reaction finished	1.7×10^7 step	48 h	-	-
	Scenario III	1	0	0	500	0.0787 mmol, (0.412 mL)
		2	3×10^6 step	8 h	1000	0.1575 mmol, (0.823 mL)

		3	6×10^6 step	16 h	1500	0.2363 mmol, (1.235 mL)
		Reaction finished	1×10^7 step	28 h	-	-
	Scenario IV	1	0	0	1500	0.2363 mmol, (1.235 mL)
		2	3×10^6 step	8 h	1000	0.1575 mmol, (0.823 mL)
		3	6×10^6 step	16 h	500	0.0787 mmol, (0.412 mL)
		Reaction finished	1×10^7 step	28 h	-	-
	Scenario V	1	0	0	300	0.0472 mmol, (0.247 mL)
		2	3×10^6 step	8 h	900	0.1418 mmol, (0.741 mL)
		3	6×10^6 step	16 h	1800	0.2835 mmol, (1.482 mL)
		Reaction finished	1×10^7 step	28 h	-	-
	Scenario VI	1	0	0	230	0.0364 mmol, (0.190 mL)
		2	3×10^6 step	8 h	693	0.1090 mmol, (0.570 mL)
		3	6×10^6 step	16 h	2077	0.3271 mmol, (1.710 mL)
		Reaction finished	1×10^7 step	28 h	-	-
	Scenario VII	1	0	0	1715	0.0675 mmol, (1.411 mL)
		2	3×10^6 step	8 h	857	0.1350 mmol, (0.706 mL)
		3	6×10^6 step	16 h	428	0.2700 mmol, (0.353 mL)

		Reaction finished	1×10^7 step	28 h	-	-
System	macro-CTA addition mode	macro-CTA addition time	Addition time point of macro-CTA		Addition amount of macro-CTA	
			Simulation	Experiment	Simulation	Experiment
			$t_{add}(i)$	$t_{add}(i)$	$n_{init}(i)$	$m_{init}(i)$
System of Fig. 9a	Benchmark	1	-	-	3000	0.4725 mmol (2.47 mL)
		Reaction finished	1.8×10^7 step	50 h	-	-
	Sample 1	10	1×10^5 step	0.28 h	300	0.04725 mmol (0.247 mL)
		Reaction finished	1.8×10^7 step	50 h	-	-
	Sample 2	30	1×10^5 step	0.28 h	100	0.01575 mmol (0.0823 mL)
		Reaction finished	1.8×10^7 step	50 h	-	-
	Sample 3	100	1×10^5 step	0.28 h	30	0.004725 mmol (0.0247 mL)
		Reaction finished	1.8×10^7 step	50 h	-	-
	Sample 4	200	1×10^5 step	0.28 h	15	0.002363 mmol (0.01235 mL)
		Reaction finished	$2.9\times10^7+$ step	$80+$ h	-	-
	Sample 5	300	1×10^5 step	0.28 h	10	0.001575 mmol (0.00823 mL)

		Reaction finished	2.9×10^{7}+ step	80+ h	-	-