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Nascent Polymerized Chain Crystallization on Surface Simulated by the Growing Chain Molecular Dynamics XIAOZHEN YANG, Institute of Chemistry — To understand nascent structure of polymerized chain on a catalyst surface, we have developed a code of growing chain molecular dynamics (GCMD), which describes aggregation behavior of growing chain with increase of repeat units during polymerization. This simulation shows that on the surface the growing chain has a nucleation process before certain chain length and an ordered structure growth process. Meantime, chain folding behavior was surprisingly observed.

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