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**Molecular Simulations of Polymer Crystallization under Nano-Confinement**[1] WENBING HU, State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University — Crystallization offers polymers under nano-scale-space confinement not only the stability of sizes and properties, but also the anisotropy of electrical conductivity, mechanical strength, and optical dichroism, etc. We make an overview on recent dynamic Monte Carlo simulations of lattice polymers performing crystallization under nano-confinement. The confined geometries include ultrathin films, nano-pores and nano-droplets of homopolymers, as well as lamellar,cylindrical and spherical self-assembled microdomains of diblock copolymers. The effects of nano-confinement on polymer crystallization can be summarized into three categories, i.e. the interface (both on enthalpy and entropy), the anisotropy of geometries and the block junction (both in its restriction and orientation). Such knowledge will facilitate our better understanding on the fabrication of nano-crystals of polymers.

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