Title: Investigating on the regulating crystallization and mechanism of Poly(L-lactic acid) by addition of low molecular-mass organic nucleating agent 有机小分子调控聚乳酸结晶及其作用机制

Abstract: Developing environment-friendly polymers is of importance national strategic. Poly(L-lactic acid) (PLLA), as a leading green thermoplastic, has exhibited great application prospects. However, the slow crystallization rate of PLLA itself restricts seriously its application and development. The introduction of a heterogeneous nucleating agent is a simple way to improve the crystallization property, but the compatibility between inorganic nucleating agents and PLLA is very poor; the organic nucleating agents often focus on a certain organic compound, as well as the unclear nucleating mechanism. In this work, the organic nucleating agents with different molecular structures are designed and synthesized, and then the crystallization promoting effects of synthesized organic nucleating agents on PLLA are investigated through nucleation activity, crystallization behavior, crystal growth, etc. The influence of the molecular structure on the induced crystallization of PLLA is determined. And according to the matching space-scale, the nucleation mechanism is further investigated via molecular dynamics simulation of PLLA and organic nucleating agent system.