

Description of Additional Supplementary Files

File name: Supplementary Movie 1

Description: Molecular dynamics simulation illustrating the cooling-driven crystallization of n-docosane, capturing its structural evolution from a disordered liquid phase to an ordered crystalline solid.

File name: Supplementary Movie 2

Description: Molecular dynamics simulation of the cooling-induced crystallization in a composite system of n-docosane with one carbon nanotube (CNT, 0.1 wt.%), showing the transition from a disordered to an ordered structure. The MD simulation reveals that a small amount of carbon nanotubes enhances the crystallization kinetics of n-alkanes through heterogeneous nucleation.

File name: Supplementary Movie 3

Description: Molecular dynamics simulation of the cooling-induced crystallization in a composite system of n-docosane with six carbon nanotubes (CNTs, > 0.5 wt. %), showing the transition from a disordered to an ordered structure. The MD simulation indicates that higher CNT loadings (> 0.5 wt. %) promotes the formation of a percolating network. This network restricts molecular mobility, consequently reducing the overall crystallinity.

File name: Supplementary Movie 4

Description: Molecular dynamics simulation illustrating the structural evolution during cooling of a blend containing n-docosane and SEBS-HDPE. The MD simulation demonstrates that the SEBS-HDPE matrix acts as a structural scaffold, forming a nanoconfinement effect on n-docosane. This effectively suppresses the leakage of the PCM in its molten state during phase transitions.

File name: Supplementary Movie 5

Description: Molecular dynamics simulation illustrating the structural evolution during cooling of a blend containing n-docosane, SEBS-HDPE, and three carbon nanotubes (CNTs, 0.1 wt.%). Both the molecular chains of polymer and n-docosane are co-adsorbed onto the CNT surface. The MD simulation indicates that molecular chains are rapidly adsorbed onto the CNT surface with only subtle conformational adjustment, forming a pre-oriented layer in the low-CNT loading system and contributing to crystallization kinetics.

File name: Supplementary Movie 6

Description: Molecular dynamics simulation illustrating the structural evolution during cooling of a blend containing n-docosane, SEBS-HDPE, and eighteen carbon nanotubes (CNTs, > 0.5 wt.%). The MD simulation demonstrates that the system with excessive CNT loading induces significant conformational rearrangement of molecular chains at the interface due to strong interfacial interactions. The percolating network restricts molecular mobility and leads to a decrease in overall crystallinity at higher concentrations (> 0.5 wt.%).