Roles of Curvature and Kink on the Thermal Transport in Polymer Chains

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With the experimental advances in making highly thermal conductive polymers, the theoretical understanding of thermal transport in polymers is still vague. In this paper, we investigated the thermal transport in a single polyethylene chain by focusing on the role of curvature and kink, which are two of the most common nano-scale features in polymers. The results show that curvature only does not affect the thermal transport in single polyethylene chains, while kinks greatly affect the thermal conductivity. The two important roles of kink on thermal conductivity of polymer chains are also discussed. A simple model is proposed to estimate the effective thermal conductivity of a single polymer chain with multiple kinks.