Significantly High Thermal Rectification in an Asymmetric Polymer Molecule Driven by Diffusive versus Ballistic Transport

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Tapered bottlebrush polymers have novel nanoscale polymer architecture. Using non-equilibrium molecular dynamics simulations, we show that these polymers have the unique ability to generate thermal rectification in a single polymer molecule and offer an exceptional platform for unveiling different heat conduction regimes. In sharp contrast to all other reported asymmetric nanostructures, we observed that the heat current from the wide end to the narrow end in tapered bottlebrush polymers is smaller than that in the opposite direction. We found that a more disordered to less disordered structural transition within tapered bottlebrush polymers is essential for generating non-linearity in heat conduction and localization asymmetry for thermal rectification. Moreover, the thermal rectification factor increased with device length, reaching as high as ~70% with a device length of 28.5nm. This large thermal rectification with strong length dependence uncovered an unprecedented phenomenon – diffusive thermal transport in the forward direction dominated by diffusons and ballistic thermal transport in the backward direction dominated by propagons. This is the first observation of radically different transport mechanisms when heat flow direction changes in the same system. The fundamentally new knowledge gained from this study can guide exciting research into nanoscale organic thermal diodes.

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