Supplementary Information for

Hydrogen-Bond Configuration Modulates Energy Transfer Efficiency in Helical Protein Nanotubes

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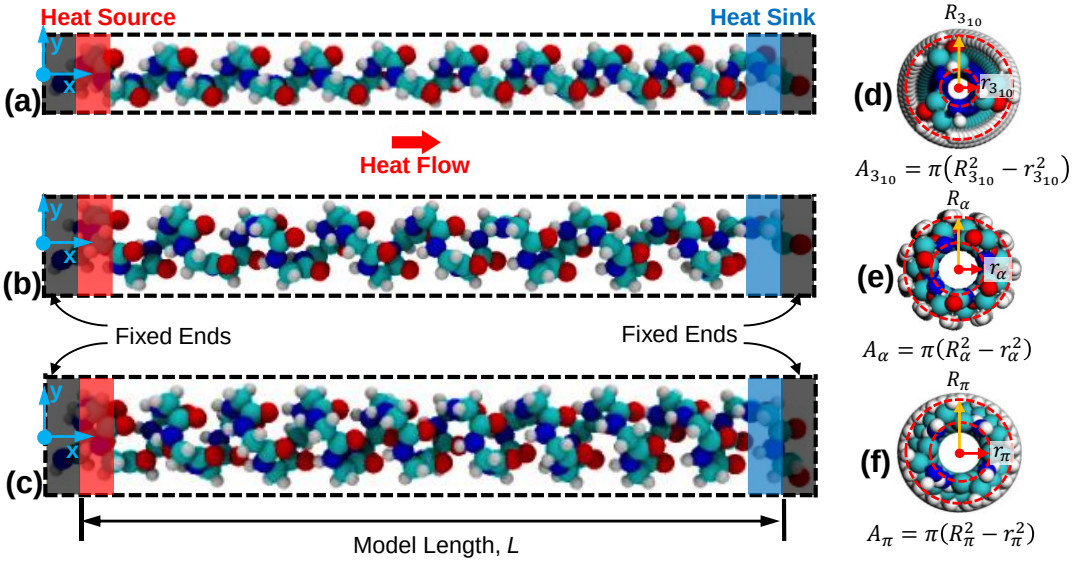

Fig. S1. Setup of the NEMD simulation for predicting thermal conductivities of the a) 3_{10}-, b) α-, and c) π-helices. Heat flow is generated by adding energy into the heat source (red region) and removing the same amount of energy from the heat sink (blue region). L is the characteristic length. The simulation cell is divided into N slabs. The two end slabs are fixed for heat insulation. Periodic boundary conditions are applied along all three directions. Cross-sectional view of the d) 3_{10}-, e) α-, and f) π-helix models. The cross-sectional area is calculated using averaged inner and outer radii of the helices.

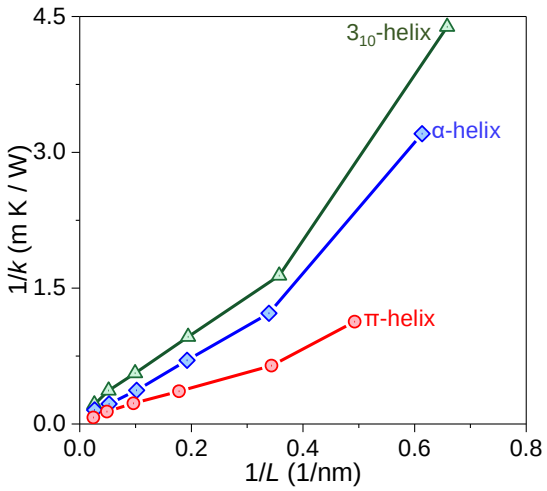

Fig. S2. Inverse of thermal conductivity versus inverse of length for the isomer helices.

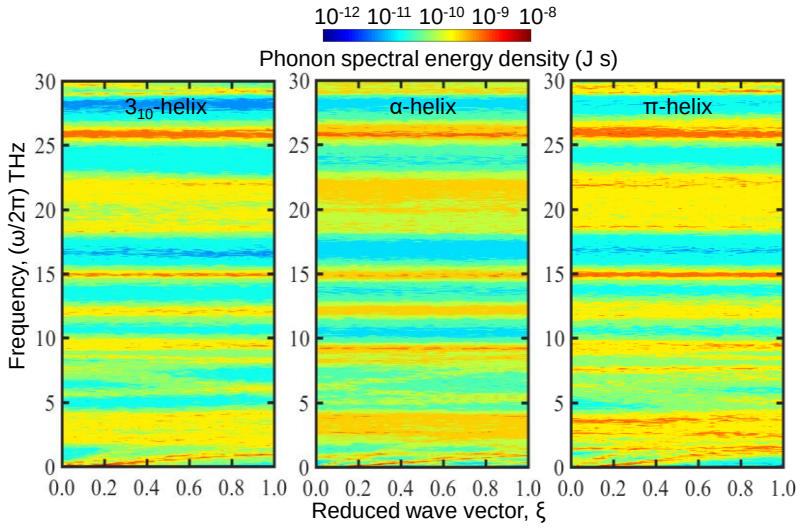

Fig. S3. Phonon spectral energy density for the three isomer helices at T = 298 K. Shading on these plots represents the magnitude of phonon spectral energy density for different phonon mode combining specific $\boldsymbol{\kappa}$ and ω.

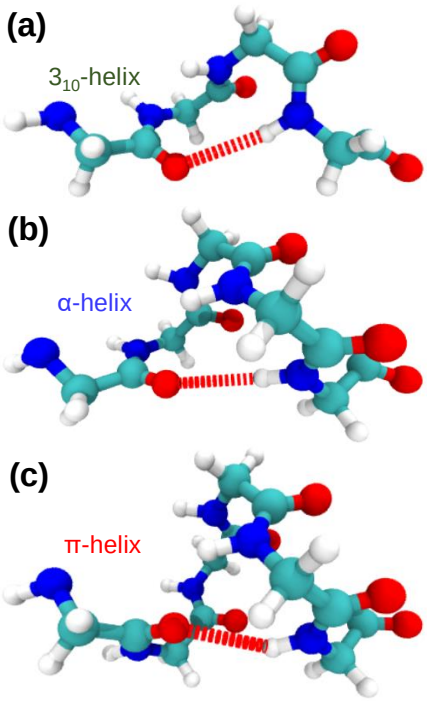

Fig. S4. Intercepted helices for DFT-based quantum-chemical analysis of H-bond: a) the 3_{10}-helix segment has four residues; b) the α-helix segment has five residues; and c) the π-helix segment has six residues.