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Theoretical Prediction of Room Temperature Thermal Superconductivity in Single Polythiophene Chains WEI LV, ASEGUN HENRY, Georgia Inst of Tech — We used molecular dynamics simulations and a new formalism for calculating the modal contributions to thermal conductivity to study individual polythiophene chains. The simulations suggest that it is possible to achieve divergent/infinite thermal conductivity (e.g., thermal superconductivity) in individual polythiophene chains. The new modal analysis method allowed for exact pinpointing of the modes responsible for the anomalous behavior, which turned out to be transverse vibrations in the plane of the aromatic rings at low frequencies $\sim$ 0.05 THz. Within the 5 ns of integration time, one mode in particular exhibits a thermal conductivity contribution greater than 100 W m-1 K-1, which is larger than many 3D bulk materials that consist of a large multitude of modes. Further investigation showed that the divergence arises from persistent correlation between the three lowest frequency modes on chains that have exact multiples of 30 unit cells in length. Sonification of the superconducting mode heat fluxes indicated distinct patterned differences between the convergent and divergent simulations, which suggests the phenomena may differ from previous models and a new explanation of the anomalous behavior may be required for polymers.

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