Understanding Divergent Thermal Conductivity in Single Polythiophene Chains Using Modal Analysis and Sonification

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Atomic Structure of Pth unit-cell

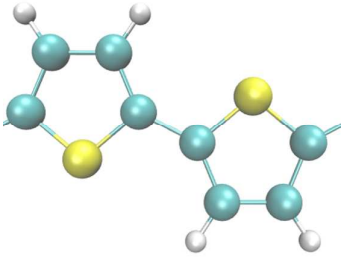


Figure s1. 1D Polythiophene chain unit cell. The green spheres represent carbon atoms, the yellow spheres represent sulfur atoms and the white sphere represents hydrogen atoms.

Relaxation time for TA-y_1 mode

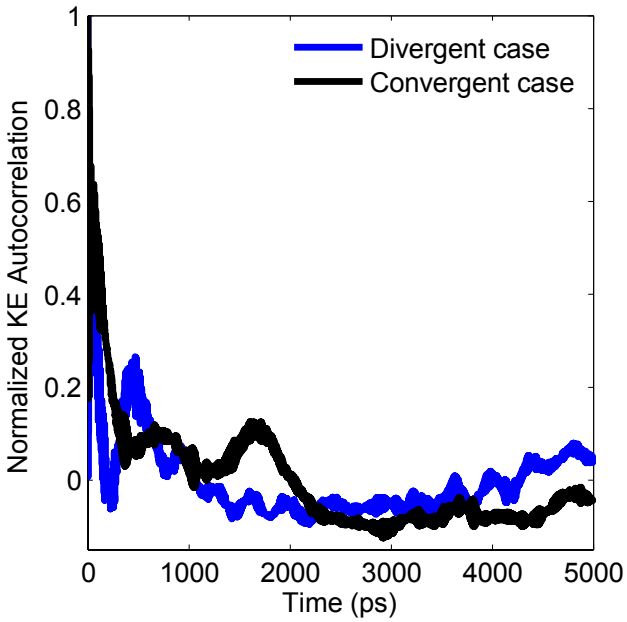


Figure s2. Normalized mode TA-y_1 kinetic energy autocorrelation functions in Pth convergent and divergent cases.

TA-y_1 mode thermal conductivity contribution

Ultimately we seek to understand the behavior of this special anomalous conducting mode (TA-y_1) in more detail. From Fig. s3, the TA-y_1 mode correlates strongly with the entire TA-y branch as indicated by the <TA-y_1·TA-y> autocorrelation shown in Fig. s4. Using GKMA, we calculated mode-mode cross correlations between the TA-y_1 mode and other modes on TA-y branch. By examining the correlation with individual modes we found that the correlation is strongest between the 3 lowest frequency modes (TA-y_1, TA-y_2, TA-y_3), where TA-y_2, TA-y_3 are second and third lowest frequency modes on the TA-y branch. In Fig. s4 it is clear that the TA-y_1 autocorrelation and its cross correlation with TA-y_2, TA-y_3 is very different for the divergent and convergent cases

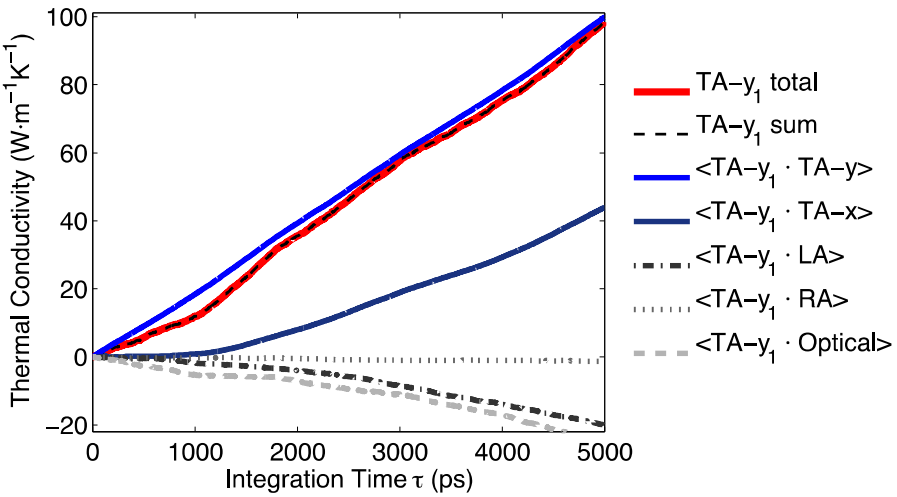


Figure s3. TA-y_1 mode thermal conductivity contribution and its correlation with different branches. Note: it includes the contribution of its symmetry mode on the same branch.

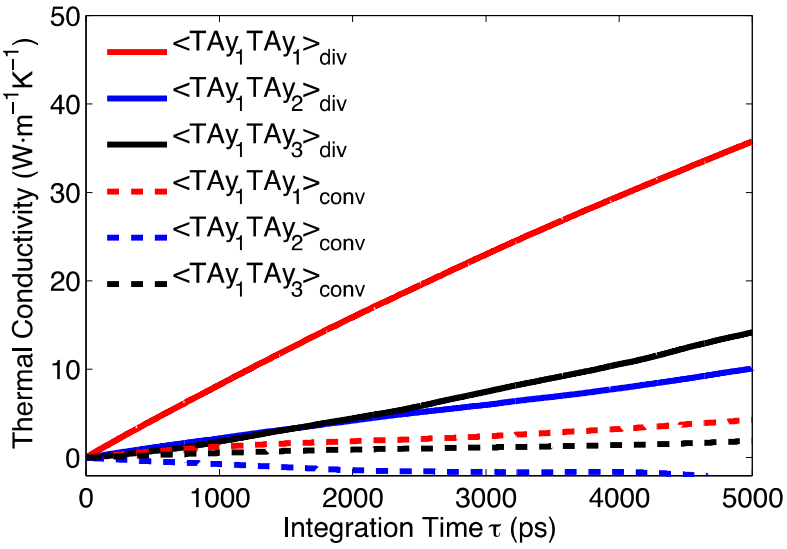
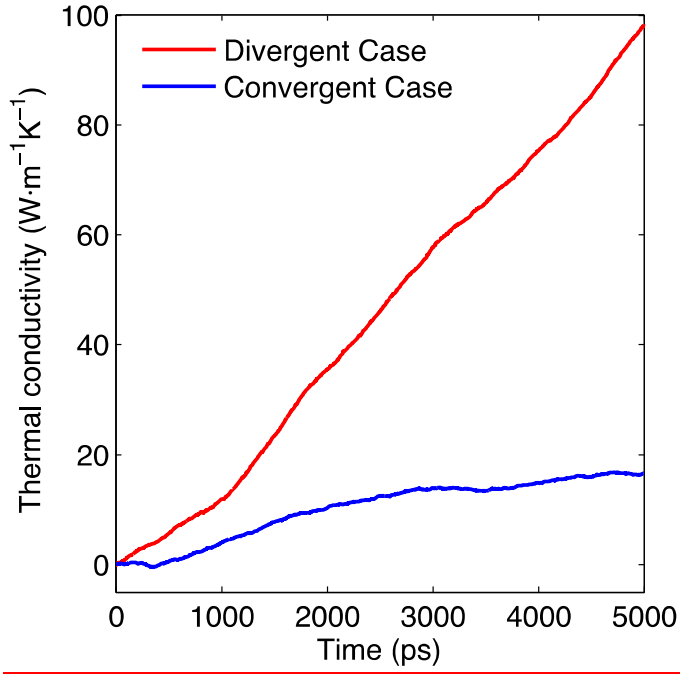


Figure s4. TA-y_1 mode thermal conductivity contribution and its correlation with TA-y_2 TA-y_3 in a divergent and convergent case.



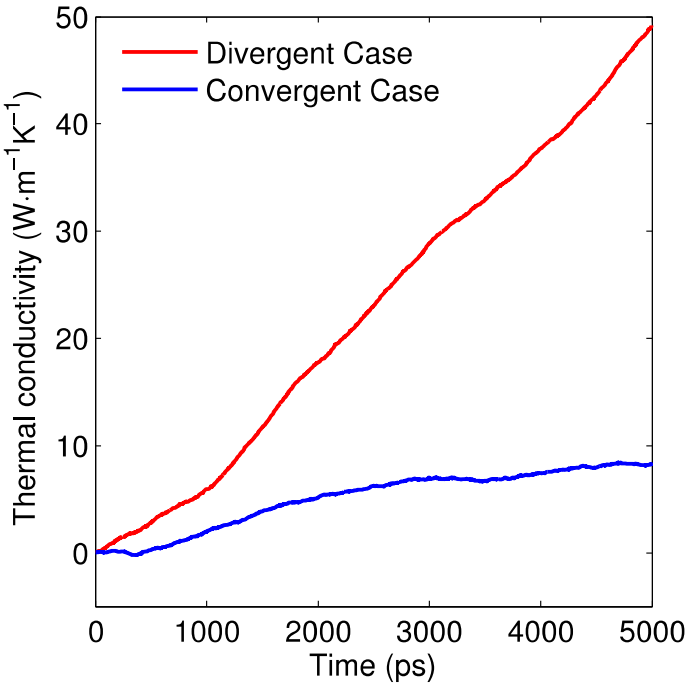


Figure s5. TA-y_1 mode thermal conductivity contribution in the divergent and convergent case.

Video files

Video file S1: Convergent TA-y_1 heat flux sonification.

Video file S2: Divergent TA-y_1 heat flux sonification.
Video file S3: Divergent TA-y_1 heat flux sonification left ear channel, convergent TA-y_1 heat flux sonification right ear channel.