Supporting Information for

Effect of Side-Chain π-π Stacking on the Thermal Conductivity Switching in Azobenzene Polymers: A Molecular Dynamics Simulation Study

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Table S1. Force field parameters related to the -N=N- connection.

Lennard-Jones Potential	ϵ (kcal/mol)			σ (Å)		
Nitrogen (N)	0.062			4.121		
Aromatic carbon (CP)	0.064			4.010		
Bond Stretching	r_0 (Å)	K_2 (kcal/mol)		K_3 (kcal/mol)	K_4 (kcal/mol)	
N=N	1.26	1400		0.0	0.0	
N-CP	1.43	720		0.0	0.0	
Angle Bending	θ_0 (degree)	K_2 (kcal/mol)		K_3 (kcal/mol)	K_4 (kcal/mol)	
CP-CP-N	120	560		0.0	0.0	
CP-N-N	116.5	650		0.0	0.0	
Dihedral Torsion	K_1 (kcal/mol)	ϕ_1 (degree)	K_2 (kcal/mol)	ϕ_2 (degree)	K_3 (kcal/mol)	ϕ_3 (degree)
CP-CP-CP-N	0.0	0.0	4.8498	0.0	0.0	0.0
H-CP-CP-N	0.0	0.0	1.7234	0.0	0.0	0.0
CP-CP-N-N	-0.6333	0.0	10.1932	0.0	0.6	0.0
CP-N-N-CP	8.3667	0.0	1.1932	180	0.0	0.0
Improper Torsion	K (kcal/mol)			χ_0 (degree)		
CP-CP-CP-N	13.0421			0.0		

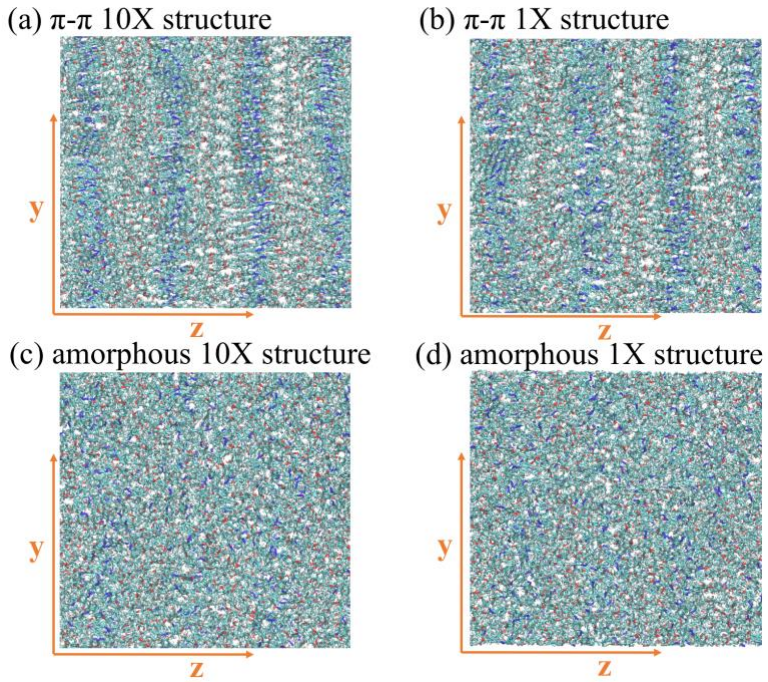
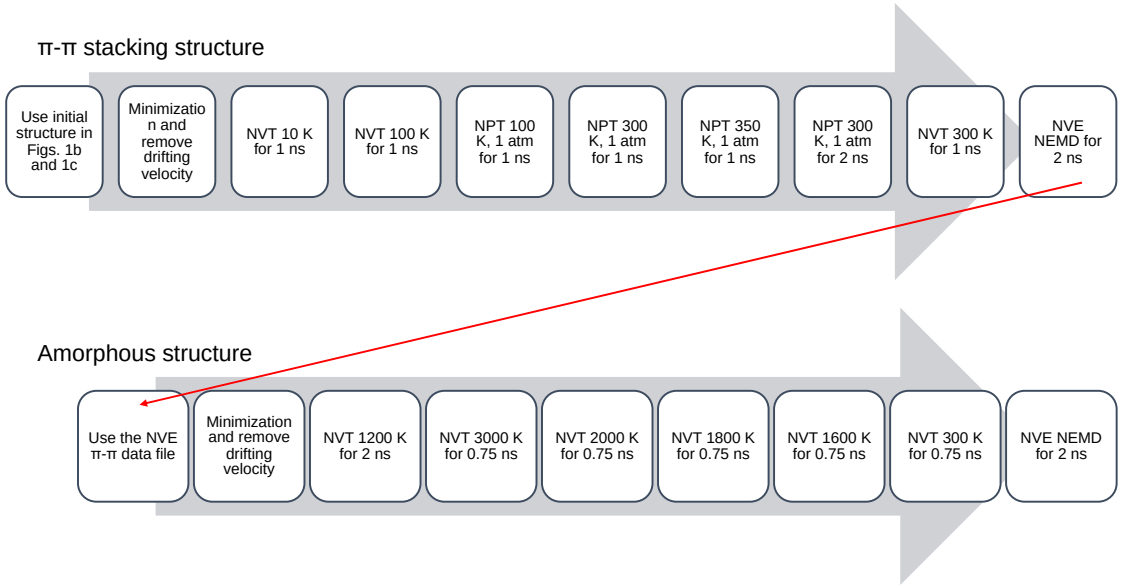


Figure S1. Polymer morphologies of (a, b) π-π stacking structures and (c, d) amorphous structures with different LJ parameter strengths, (a, c) 10X and (b, d) 1X.



Scheme S1. Simulation procedure for relaxing the polymer model and thermal conductivity calculations.

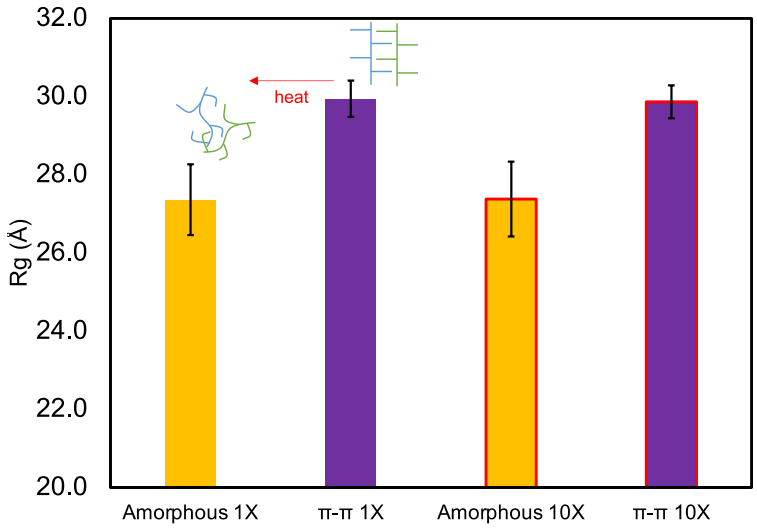


Figure S2. Polymer radius of gyration (R_g) comparison between the 4 polymer models: amorphous 1X vs amorphous 1X, and π-π 10X vs amorphous 10X.

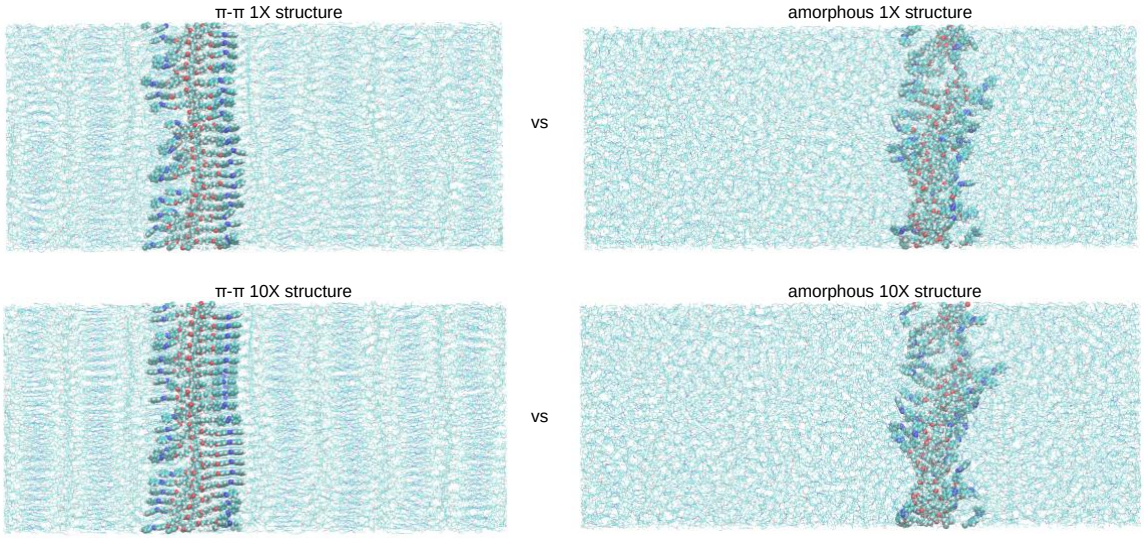


Figure S3. Comparison of polymer schemes: π-π 1X vs amorphous 1X, and π-π 10X vs amorphous 10X. In the amorphous structures, the side-chains are more entangled, but the polymer backbone conformations are similar to those of the π-π stacking structures.

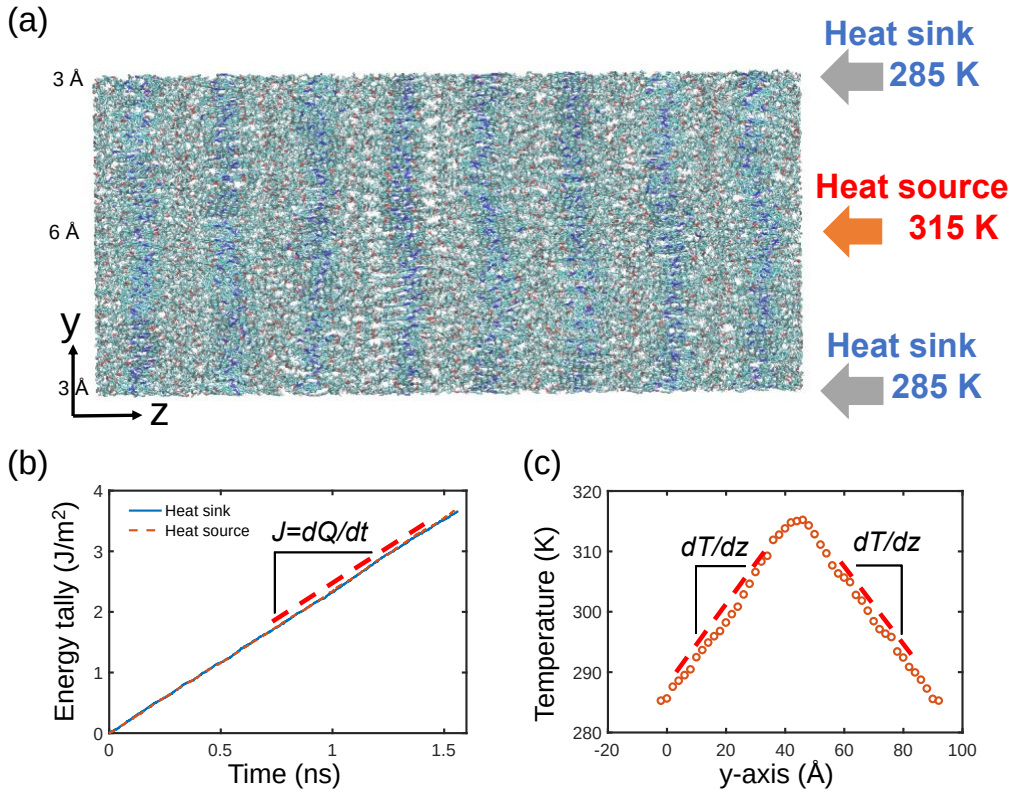


Figure S4. NEMD method for calculating thermal conductivity in the y-axis. (a) Scheme of the simulation model. (b) Heat flux calculation. (c) Temperature gradient calculation.