Electronic Supplementary Material (ESI) for Nanoscale Advances.

Supplementary Information

Aligned Structure of Mesogenic Motifs in Epoxy Resin and Their Effects on Thermal Conductivities

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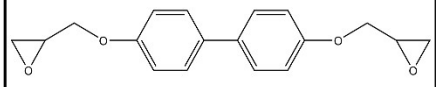
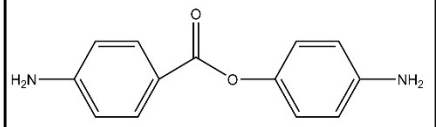
Several MD simulations were conducted with simple EH pair which the molecular structure depicted in **Table S1** to test simulation parameters. The same procedure explained in the main text was applied to get the TC of crosslinked structure. The OPLS-AA force field with partial charges tabulated in Moltemplate was used in this case. At first, the box length of the simulation was determined from HCACF convergence test with the EH pairs which are depicted in **Fig. S1 (a)** where crosslink ratio p was 0.7 and the result was from the single MD run result. Also, HCACF results from the EH7 and the EH8 of the main text are provided in **Fig. S1 (b)** for comparison among different EH pairs. The crosslink ratio and cut-off distance used for searching functional group pairs are presented in **Fig. S2**. The TC values obtained from different network structures are plotted in **Fig. S3** which were from independent network constructing procedure. The TC dependency on p are shown in **Fig. S4**. The parameters tested by 20 runs of repeated simulations with different initial velocities for more reliable results. All TC values were also scaled down with the scale factor S = 0.76.

Table S1 Molecular representation of EH pair to parameter test of MD simulation

Epoxy (E)	
Hardener (H)	

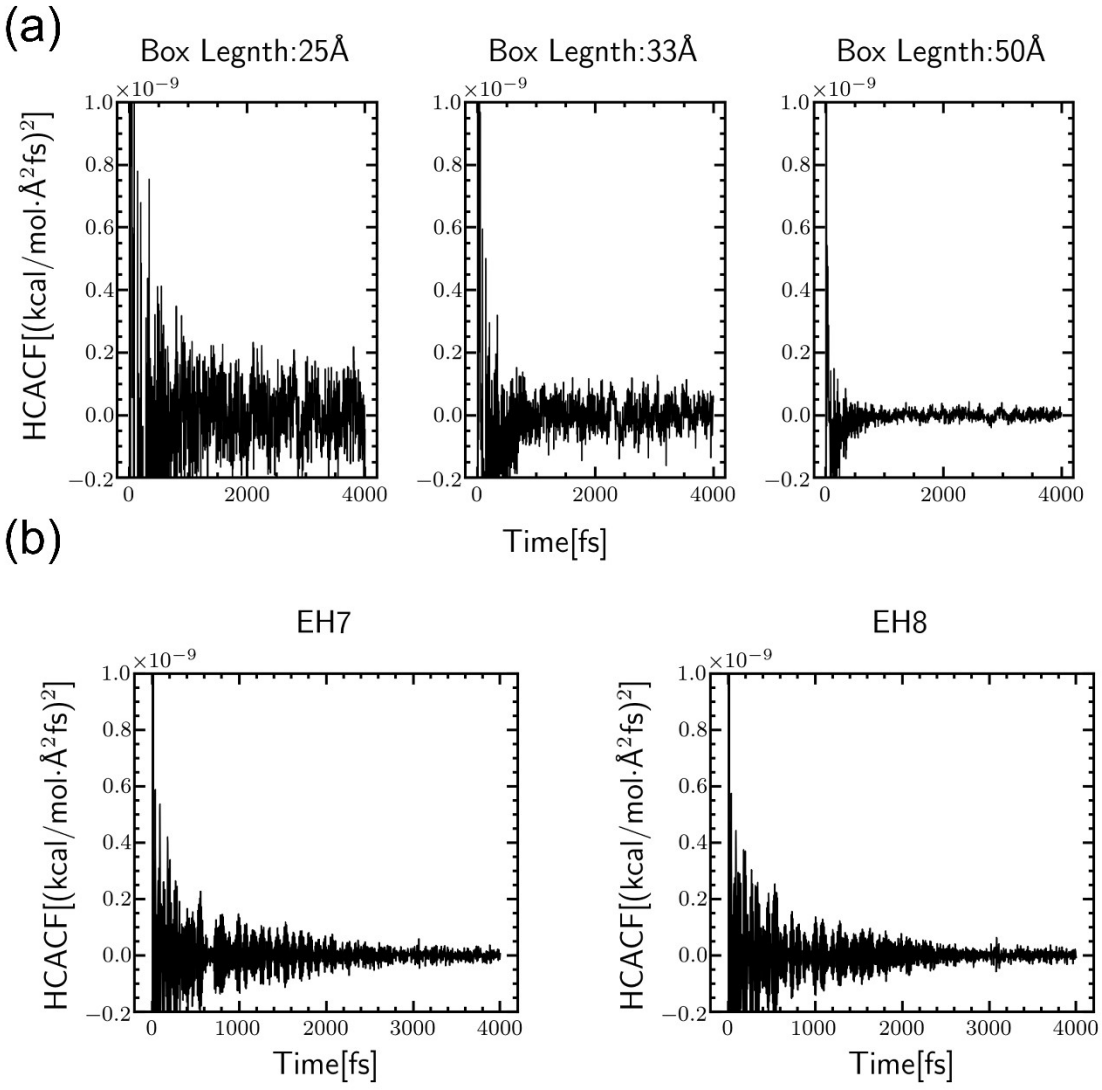


Fig. S1 HCACF plots with different box lengths. (a) HCACF plots from results of EH7 and EH8. (b)

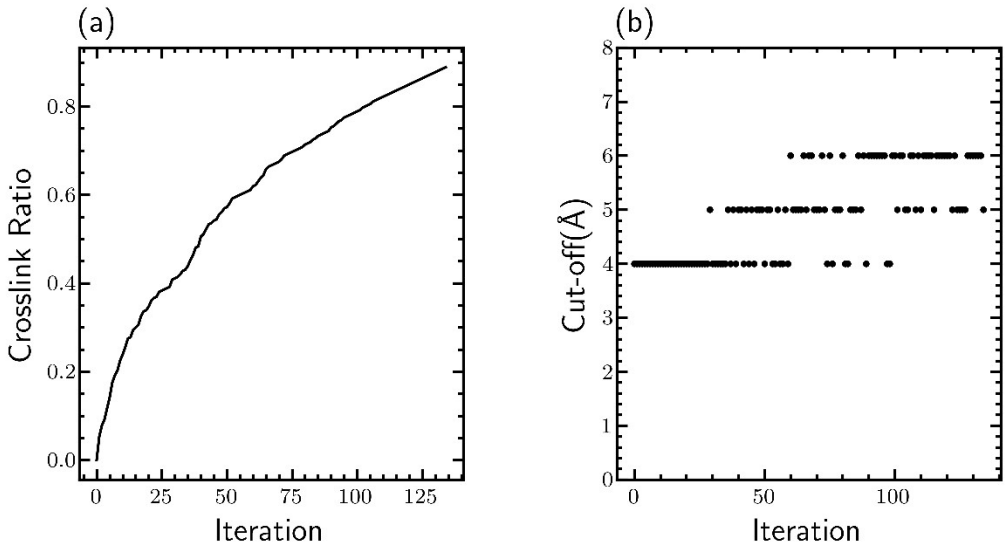


Fig. S2 Crosslink ratio (a) and used cut-off distance (b) according to the number of iterative MD runs. The crosslinked ratio was 0.7 and the box size was 50Å.

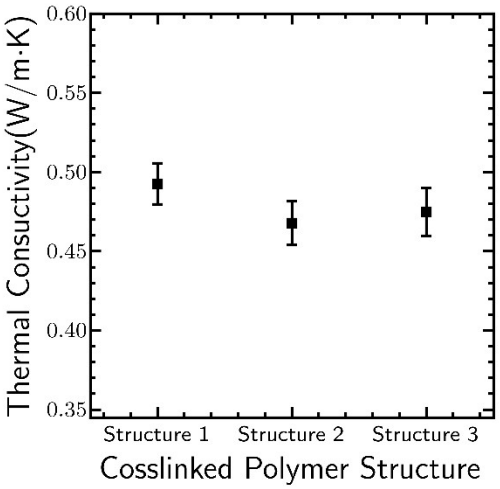


Fig. S3 TC variation among the independently formed crosslinked structure. Each structure was made following **Figure 1**. The crosslinked ratio was 0.7 and the box size was 50Å.

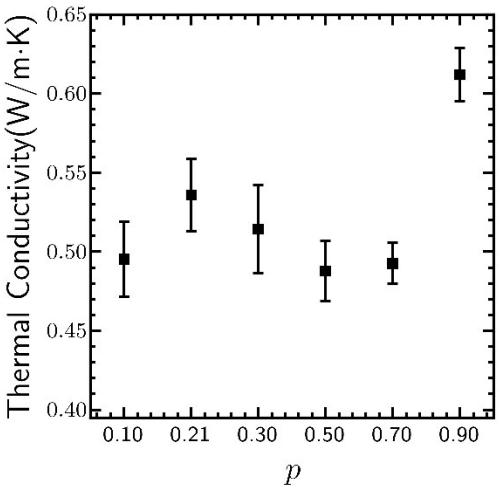


Fig. S4 TC according to crosslinked ratio p where the box size was 50 Å. The error bars are from the 95% confidence interval range of independent runs.

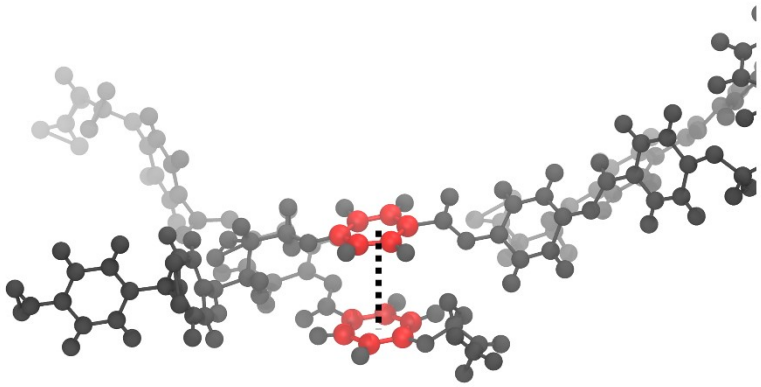


Fig. S5 Representative snapshot of aligned aromatic groups in the crosslinked polymer. The aligned aromatic groups are colored red and with the dashed line where only part of near and connected with the groups are depicted.

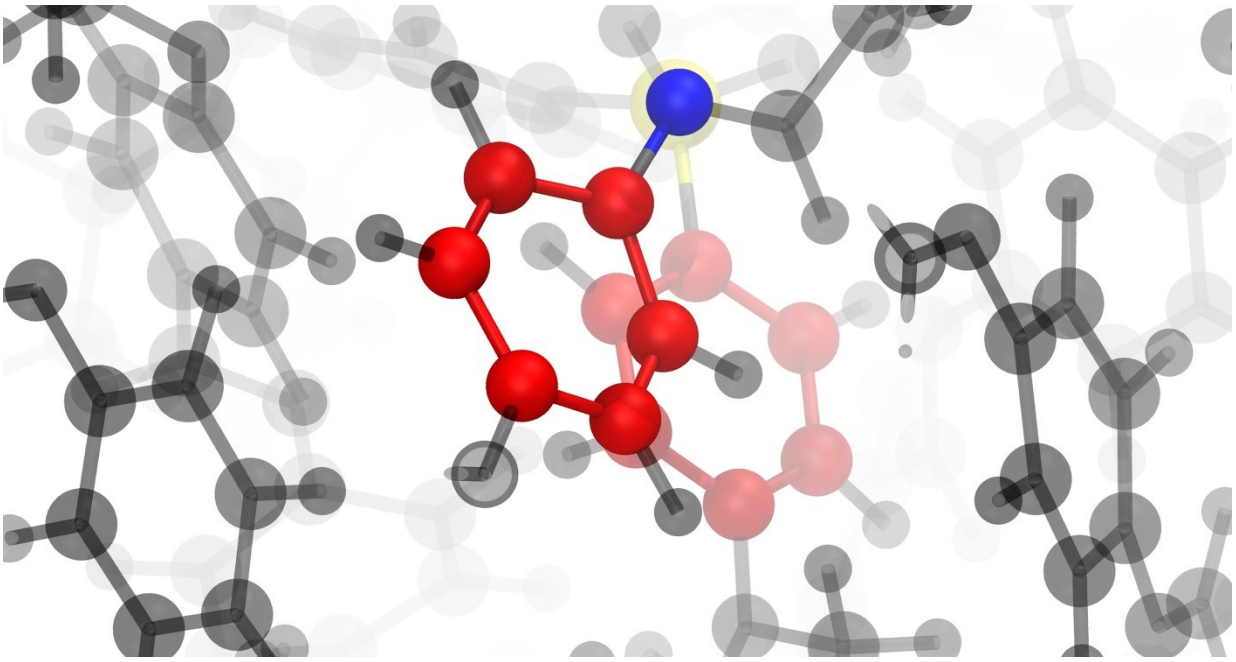


Fig. S6 Representative snapshot of the aromatic group pair(red) in EH5 which are distanced by the intermediate distance(5.5 Å) due to coordination of the nitrogen(blue) and sulfur(yellow).