Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information to:

Designing high thermal conductivity of cross-linked epoxy resin via Molecular Dynamics Simulation

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An epoxy resin, E51, was obtained from Dalian Liansheng Trading Co., Ltd . polyether amine (D230, D400 and D2000) was used as a curing agent for E51. We use three different molecular weight (chain length) curing agents to cure epoxy at room temperature.

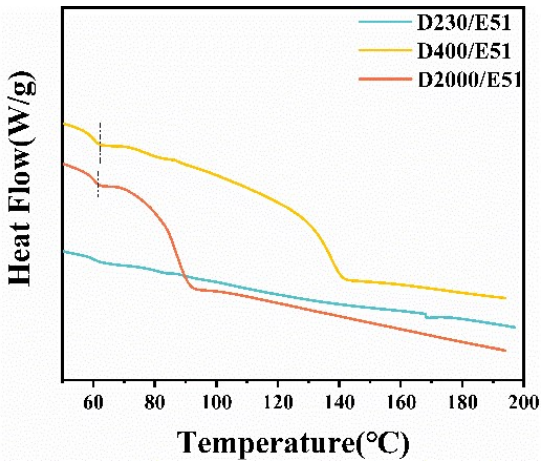

Figure S1. DSC curve for three types of curing agent cured epoxy resin

Figure S1 shows the dynamic DSC thermograms of three systems obtained at a heating rate of 10°C/min. The glass transition temperature of D230 cured epoxy resin is 63 ° C, while that of D400 cured epoxy resin is 60 ° C. The glass transition temperature of D2000 is too low to be observed in this graph. It can be seen that the effect of the polyether amine-based curing agent on the glass transition temperature of the cured epoxy resin basically accords with the decrease of the molecular weight (chain length) of the curing agent.

At the same time, we compared the effects of two different mutual attractive interactions, (r_{cutoff} =2.24σ and r_{cutoff} =2.5σ) on the thermal conductivity of the system. Taking 90% cross-linking systems with multi-functional groups of the curing agent as examples, we have calculated the thermal conductivity of those systems with r_{cutoff} =2.24σ and r_{cutoff} =2.5σ, respectively. As shown in Fig.2, compared with the original TC employing r_{cutoff} =2.24σ, switching to r_{cutoff} =2.5σ results in a tiny increase in the TC. However, the overall trend of TC induced by the number of functional groups remain unchanged. At the same time, using r_{cutoff} =2.24σ can improve the computational efficiency.

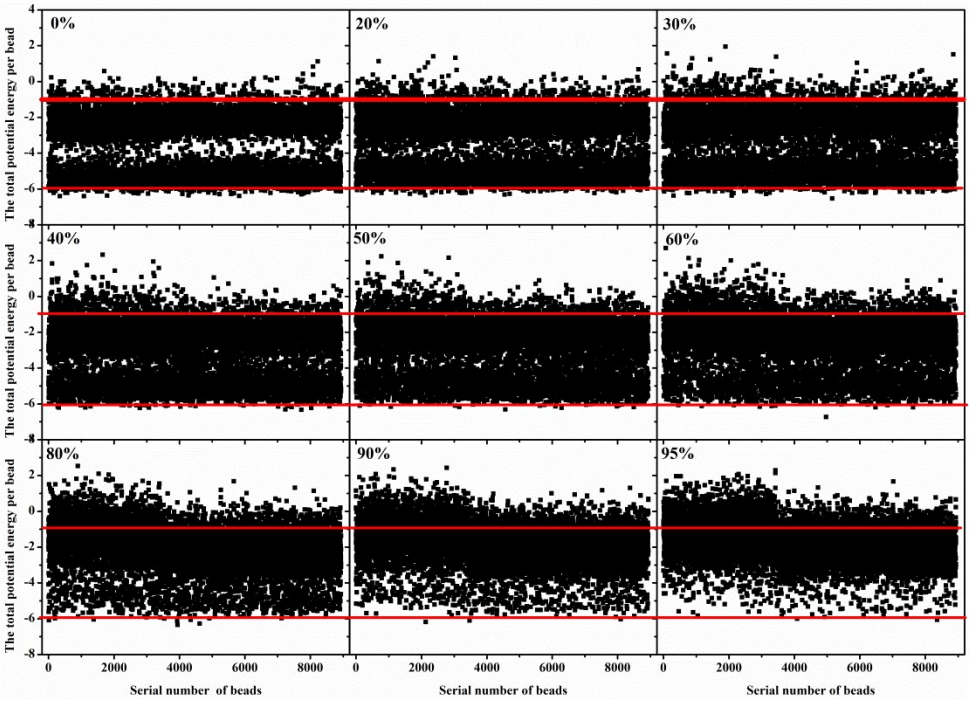

Figure S2. The total energy of each bead at different crosslinking degree

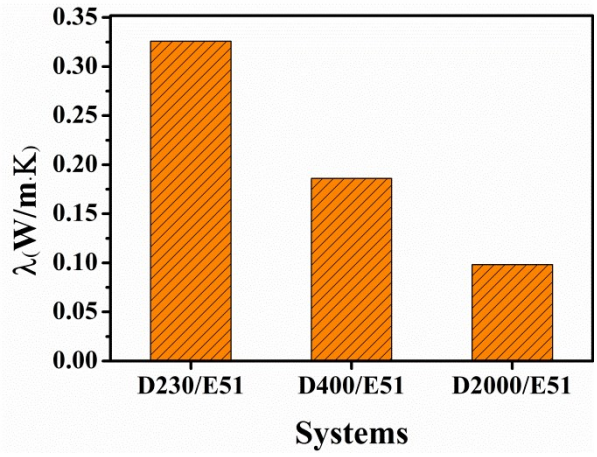

Figure S3. Effect of the different curing agents on the thermal conductivity of the epoxy resin

Figure S3 shows the Effect of the different curing agents on the thermal conductivity of the epoxy resin. The thermal conductivity of three systems is seen to decrease with the increasing the molecular weight (chain length) of the curing agent.