Modeling the formation and thermomechanical properties of polybenzoxazine thermosets

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Supplementary Information

The $T_g$ is very often estimated through the volume versus temperature curves with similar slope variation analysis. However the values obtained by the two methods differ by about 35 K; the density-temperature method adopted here provides results in better agreement with experiment, as also noticed by other groups.s1,s2 Another point to note is that the cooling rates used in simulations are multiple orders of magnitude higher than in the experimental measurements. A priori this should affect the values of calculated $T_g$. In similar works the error between simulation and experimental $T_g$ values are often corrected by Wiliams-Landel-Ferry (WLF) equation which takes into account the cooling rate differences.s3 However, in this work the cooling rate does not seem to affect our results; all the studied structures can be considered at equilibrium after 300 ps; Fig. S1. This was verified by launching simulations for monomer-systems at different cooling time steps: 200 ps, 400 ps, 800 ps (see Figure S2). The results gave the same value of $T_g$ for all simulation boxes.

Fig. S1 Density as a function of time for P-pPDA (conversion 0 % and 90 %) at 300 and 800 K.
Fig. S2 Density as a function of the temperature for different cooling rates of the P-pPDA monomer.

