Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Simple and Convenient Mapping of Molecular Dynamics Mechanical Property Predictions of Bisphenol-F Epoxy for Strain Rate, Temperature, and Degree of Cure

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S1. Sensitivity of experimental modulus scatter on the mapping factor

To study the effect of the data scatter from Figure 3a on the viscous response mapping factor, the 95% confidence interval was calculated on the data presented in Figure 3a, as shown in Figure S1(a). The factor $f_\alpha(\alpha)$ was determined at 27˚C for both the upper and lower limits of the 95% confidence interval. The corresponding mapping to the Young's modulus is shown in Figure S1(b). Figure S1(b) shows that the results of the scatter from Figure 3a affect the magnitude of the Young's modulus, but on the overall trend. It is important to note that there is limited data in the literature for modulus of this material at high strain rates. The availability of additional data would ideally reduce the confidence interval limits and provide more precise predictions.

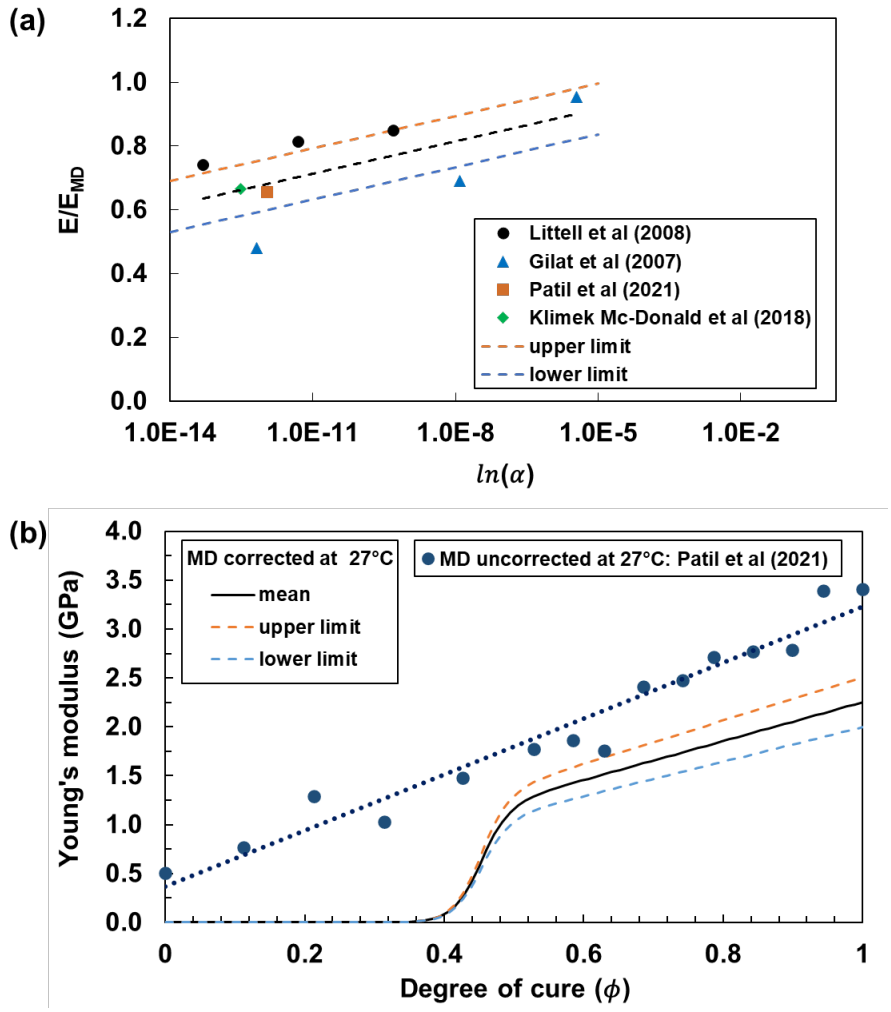

Figure S1 – (a) Normalized Young's modulus of DGEBF/DETDA epoxy as a function of applied normalized strain rate determined experimentally with 95% confidence intervals, (b) Plot of MD uncorrected (open circles) and corrected (solid lines) Young's modulus vs degree of cure for 27˚C for the curve fit shown in (a) and the 95% confidence interval lines.