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

Atomistic Explorations of Mechanisms Dictating the Shear Thinning Behavior and 3D Printability of Graphene Flake Infused Epoxy Inks: Supplementary Materials

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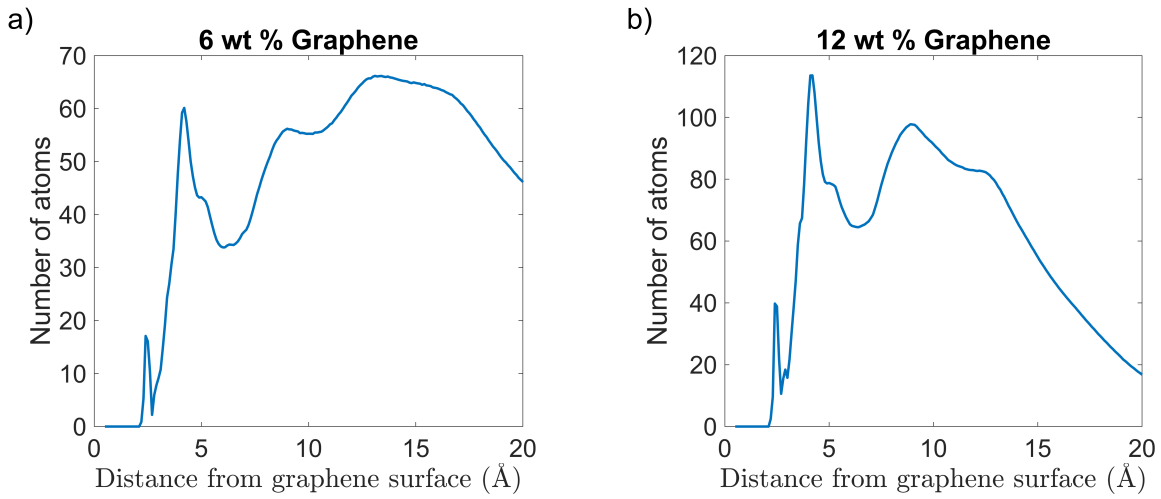

Figure S1. Histogram distribution of the shortest distance between a polymer atom and the graphene surface for a) 6wt% graphene infused epoxy and b) 12wt% graphene infused epoxy inks. A bin size of 0.1 Å was used to generate these distribution plots.

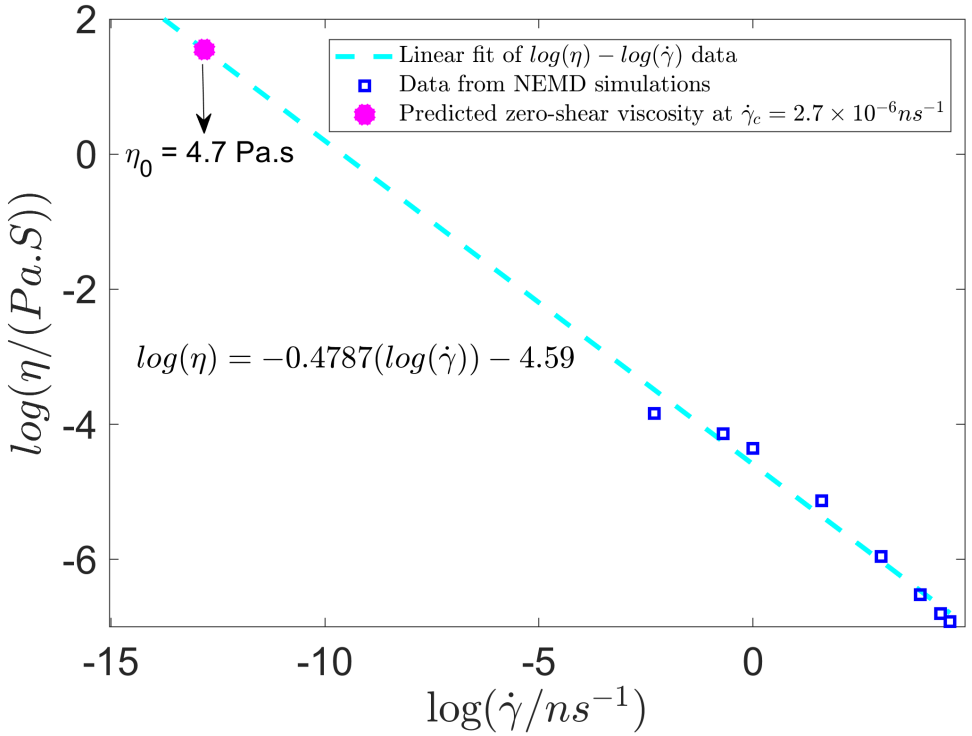

Figure S2. Linear regression of log(η) vs log($\dot{\gamma}$) data using the standard power-law model for shear-thinning regime written as $\eta(\dot{\gamma}) = A\dot{\gamma}^n$. The exponent *n* was found to be -0.4787 for our NEMD simulation data. Using the critical shear rate of $\dot{\gamma}_c$ = 2700 s^{-1} for pure epoxy (Epon 862 with Epikure curing agent W) reported in previous experimental studies,[1] our power-law model predicts a zero-shear viscosity of 4.7 Pa.s which is close to the experimental value of 3.93 Pa.s.[1] Since the power-law model is only applicable to the shear-thinning regime, the extrapolation should only be performed until the critical shear rate below which the Newtonian regime starts and the viscosity remains independent of the shear rate.

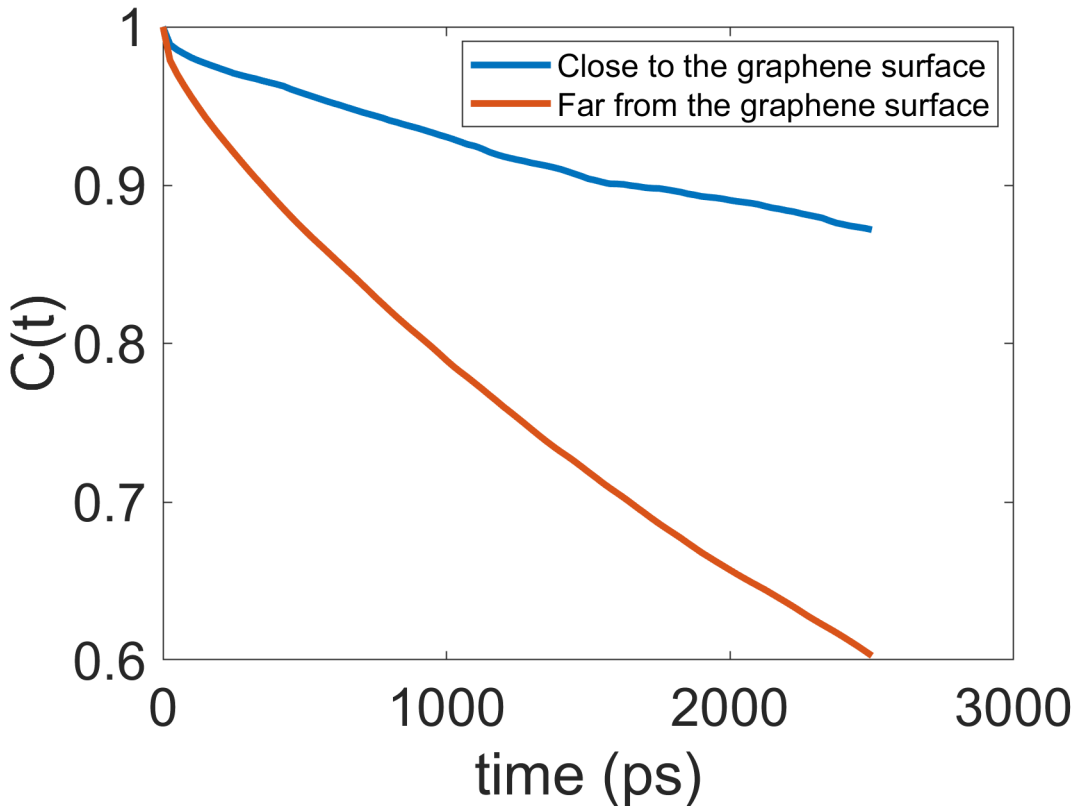

Figure S3. Re-orientational correlation function of the end-to-end vectors of bisphenol F molecules close to (in the first parallel layer of molecules adsorbed to the graphene surface) and far away (outside the first parallel layer of molecules) from the graphene surface in 6wt% graphene infused epoxy. Here, we can clearly see that the correlation function decays much faster for molecules far from the graphene surface compared to the ones adsorbed on the graphene sheet.

S1. FORCE FIELD PARAMETERS

Table S1.

Atom type	ε (Kcal/mol)	σ (Å)
c_2	0.0540	4.0100
c_3	0.0540	4.0100
c_3h	0.0540	4.0100
cp	0.0640	4.0100
hc	0.0200	2.9950
hn	0.0130	1.0980
nb	0.0650	4.0700
o_3e	0.2400	3.5350
oc	0.2400	3.5350
cp (graphene)	0.0640	4.0100
hc (graphene)	0.0200	2.9950

The charges on all the atoms of DGEBF and DETDA, which were obtained from the PCFF parameter set as a sum of bond increments, are shown in figure S4.

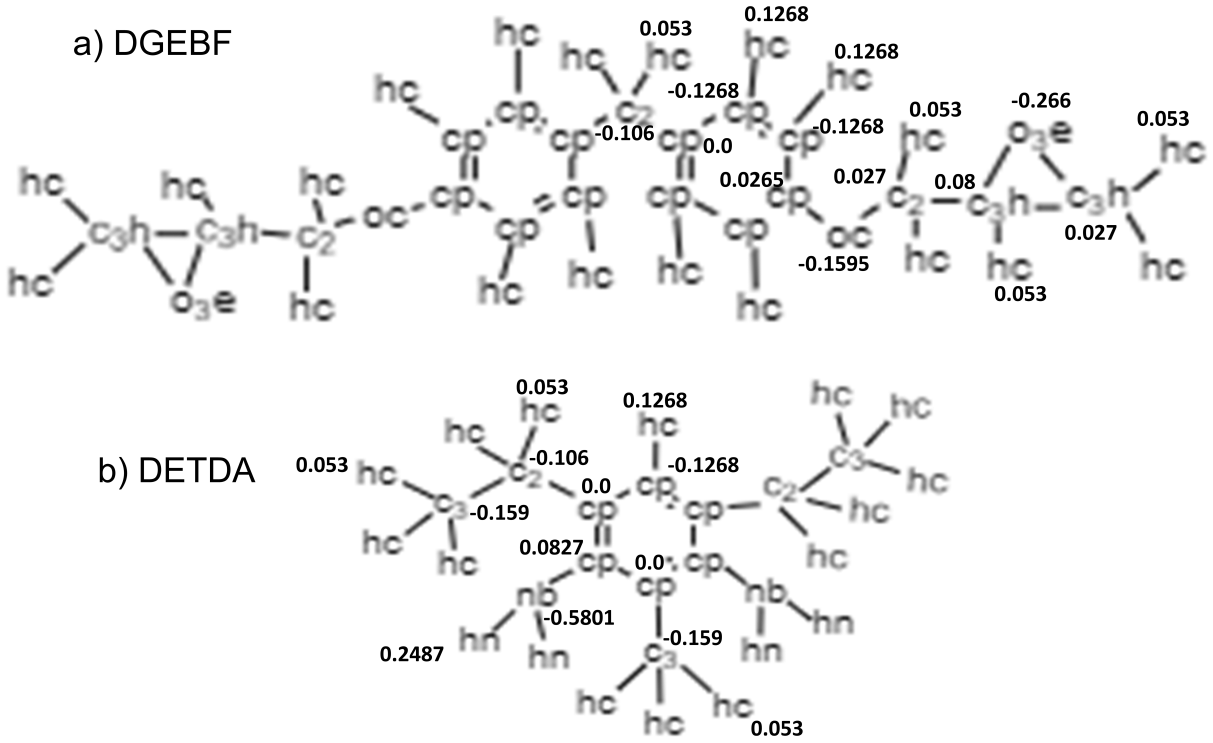

Figure S4. Atom types and the corresponding charges (in the units of electron charge (e)) of all the atoms in DGEBF and DETDA. Charges on symmetric atoms are only labeled once.

References:

1. Zhu, J., Wei, S., Ryu, J., Sun, L., Luo, Z., & Guo, Z. (2010). Magnetic epoxy resin nanocomposites reinforced with core− shell structured Fe@ FeO nanoparticles: fabrication and property analysis. *ACS Applied Materials & Interfaces*, *2*(7), 2100-2107.