Supplementary Information

Bio-based epoxy functionalized MQ silicone resins: from synthesis to toughened epoxy composites with good mechanical properties, thermal resistance and transparency

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1) GPC curves of H-MQ, EG-MQ, AG-MQ

2) Molecular simulation

3) TEM images of EG-MQ-20% thermosets

4) Optical image of the EG-1.2MQ-20% specimen during the flexural test

5) High Resolution SEM images of EG-0.8MQ-20% and EG-1.0MQ-20%

1. GPC curves of H-MQ, EG-MQ, AG-MQ

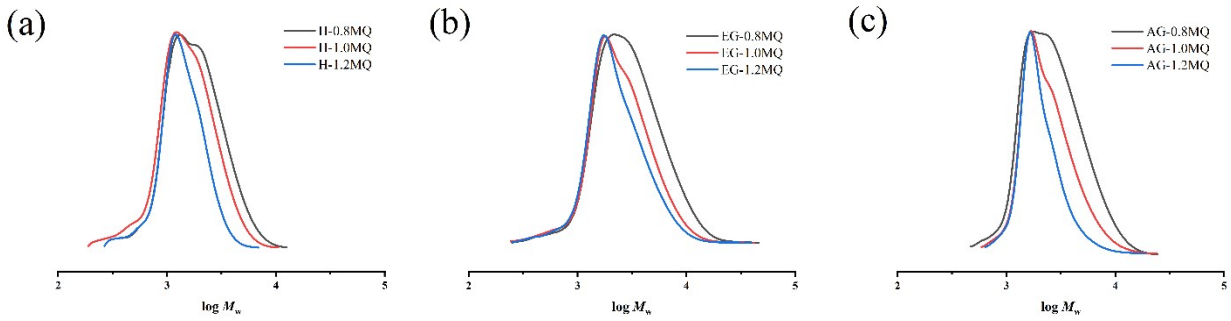

Figure S1. GPC curves of H-MQ (a), EG-MQ (b), and AG-MQ (c) in different M/Q ratios.

2. Molecular simulation

2.1 Establishment of molecules

All molecules were conducted using the Polymer Build Module, the structure of epoxy MQ silicone resins are established from the H-MQ structures as shown in Figure S2. All structures were geometry optimized using the COMPASS II force field. Each amorphous cell was constructed with 10 same molecules (DGEBA/IPDA was constructed with 10 DGEBA and 5 IPDA molecules).

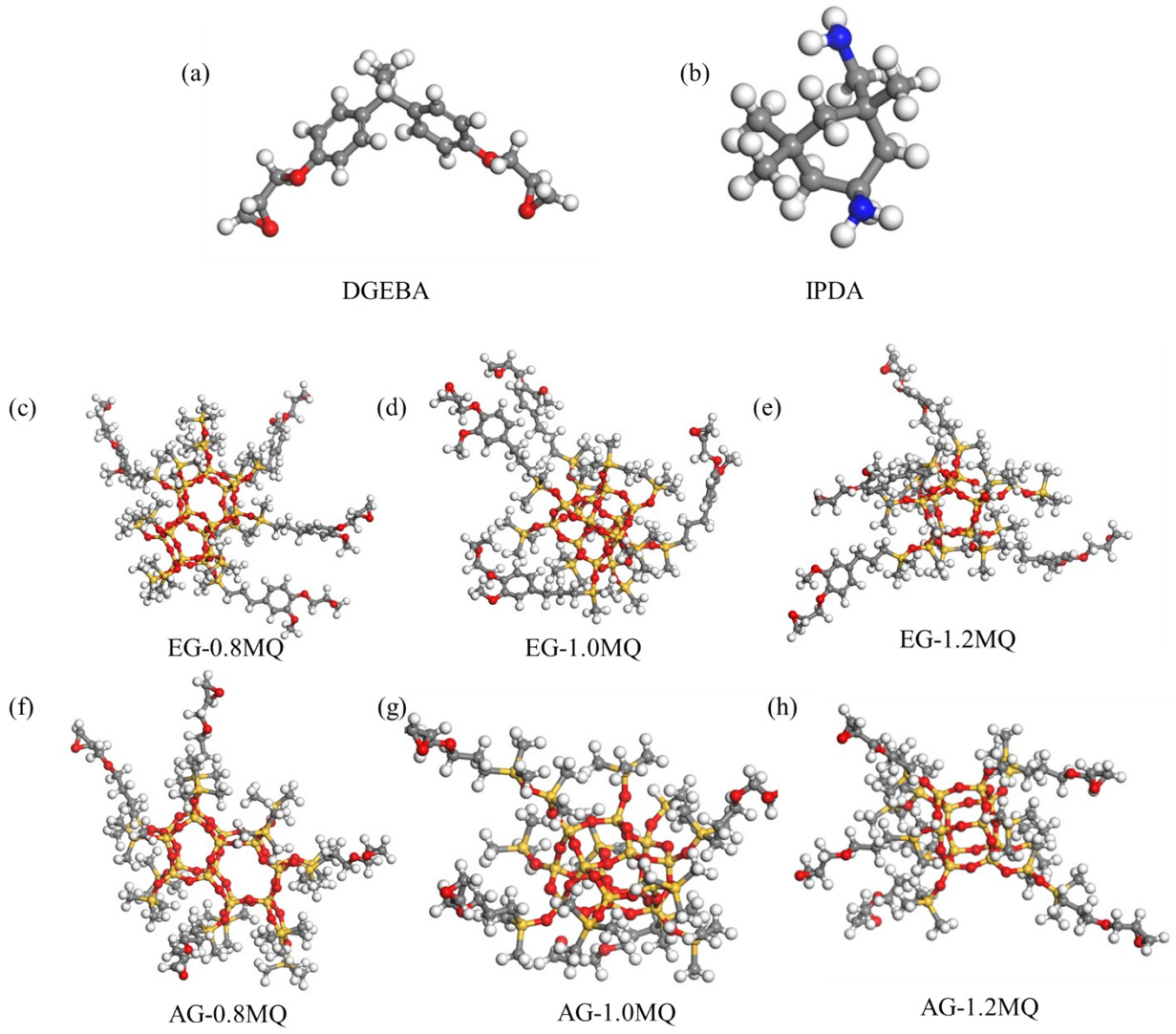

Figure S2. Molecular structure of DGEBA, IPDA, and epoxy MQ silicone resins.

2.2 MD simulation

Following this, the MD simulations were carried out in two steps: the equilibration step and the production step. The goal of the equilibration step is to thermodynamically relax the stress points and density inhomogeneities in the system. The step involves geometry optimization followed by 10ps of NVT dynamics with a 0.5ps time step at the given simulation temperature. This is followed by a temperature cycle from a high temperature (600 K) to a low temperature (300K)

using the short NVT and a longer NPT calculation. Next step is density equilibration (50 ps duration) involving multiple restarts of an NPT calculation at the target pressure. Convergence is when the differences in block densities falls below the specified value which was 0.04 (density difference) in this case (Figure S3). The final cohesive energy density and solubility parameter can be calculated from the Forcite-CED simulations, the data are list in Table S1.

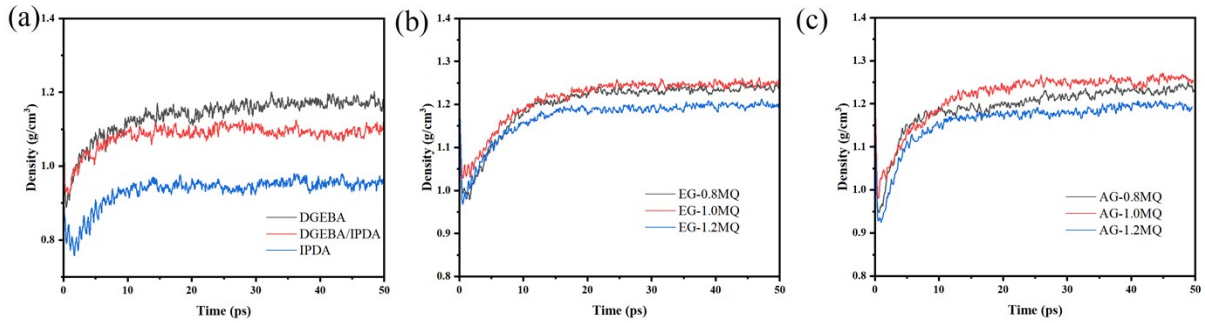

Figure S3. Molecular density (a) DGEBA, IPDA and their mixture (b) EG-MQ (c) AG-MQ.

Table S1. Cohesive energy density and solubility parameter.

	Cohesive energy density ($J/m^3 \times 10^8$)	**Solubility parameter $(J/cm^3)^{1/2}$**	**van der Waals solubility $(J/cm^3)^{1/2}$**	**Electrostatic solubility $(J/cm^3)^{1/2}$**	**Other solubility $(J/cm^3)^{1/2}$**	**Experiment density (g/ml)**	**Predicted density (g/ml)**
DGEBA	4.29	20.7	19.9	4.9	3.2	1.16	1.17
IPDA	3.44	18.6	17.0	6.8	2.8	0.92	0.95
DGEBA/IPDA	4.18	20.4	19.0	6.9	3.1	1.10	1.10
EG-0.8MQ	1.93	13.9	13.3	3.0	2.9	1.21	1.25
EG-1.0MQ	2.15	14.7	14.0	3.3	3.0	1.20	1.24
EG-1.2MQ	2.36	15.4	14.8	3.1	3.1	1.15	1.19
AG-0.8MQ	0.85	9.2	8.4	2.6	2.8	1.21	1.23
AG-1.0MQ	1.25	11.2	10.3	3.1	2.9	1.20	1.25

AG-1.2MQ	1.62	12.7	12.2	2.1	2.8	1.17	1.20

3. TEM images of EG-MQ-20% thermosets

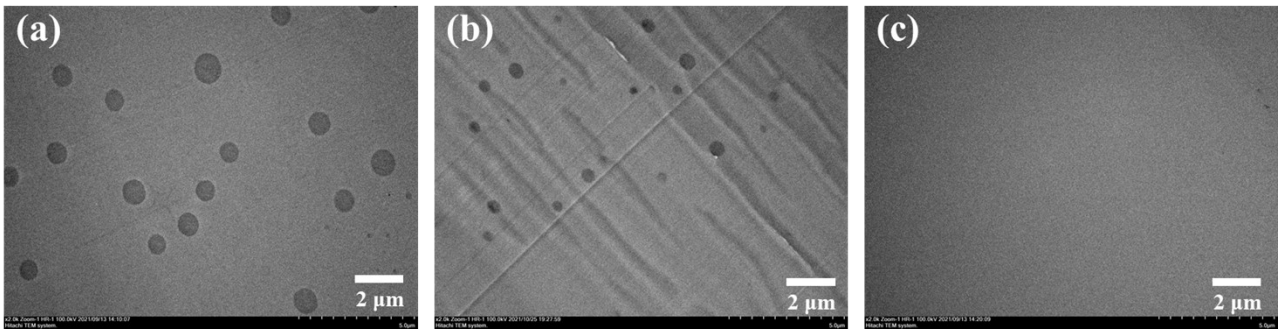

Figure S4. TEM images of (a) EG-0.8MQ-20% (b) EG-1.0MQ-20% (c) EG-1.2MQ-20%.

4. Optical image of the EG-1.2MQ-20% specimen during the flexural test

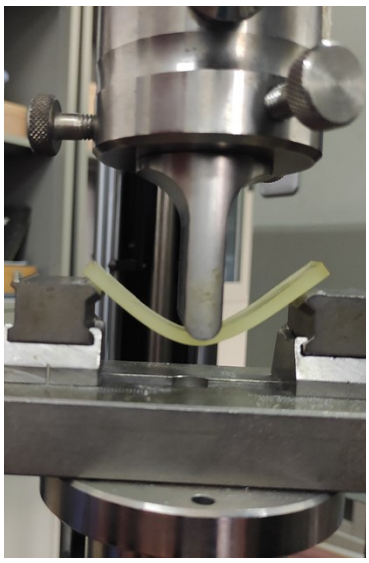

Figure S5. Optical image of the EG-1.2MQ-20% specimen during the flexural test.

5. High Resolution SEM images of EG-0.8MQ-20% and EG-1.0MQ-20%

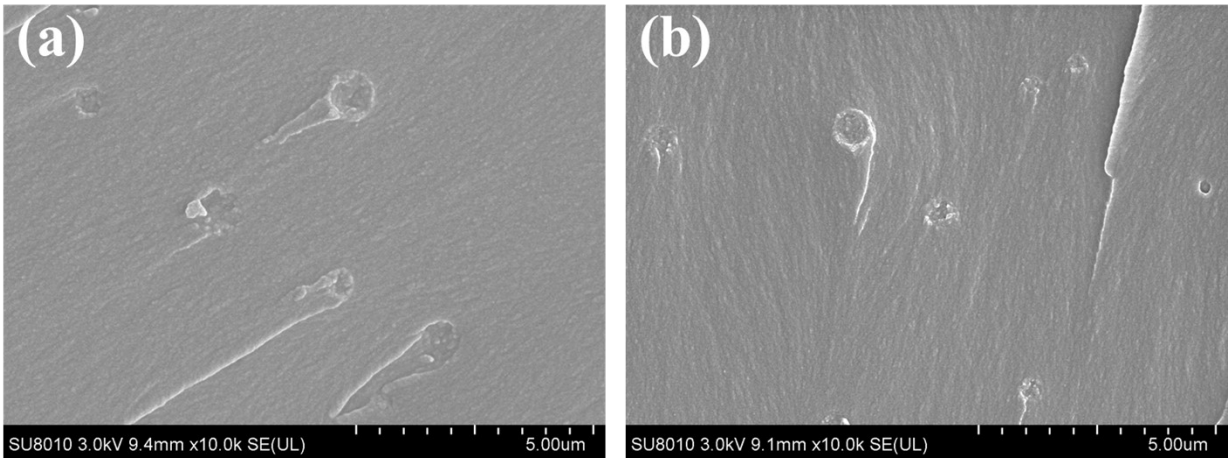

Figure S6. High Resolution SEM images of (a) EG-0.8MQ-20% and (b) EG-1.0MQ-20%.