# Optimizing Dielectric, Mechanical, and Thermal Properties of Epoxy Resin through Molecular Design for Multifunctional Performance

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## 1 Structure of epoxy resin

In this study, the amine/epoxy resin system consisting of resin solution (ARALDITE® LY 5052) and amine hardener (ARADUR® 5052 CH) are used. The curing reaction in this system, along with the resulting crosslinked polymer network[1,2], is illustrated in **Figure S1**.

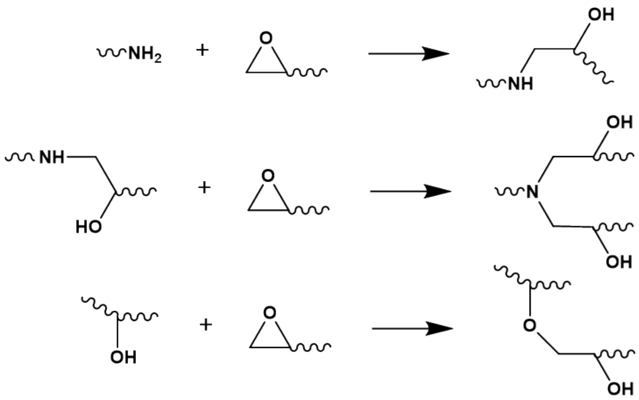

**Figure S1.** Main reaction between epoxy resin and hardener used in this study.

## 2 Dimensions of tensile specimens.

The tensile measurement was conducted based on ASTM D638 test standard[3]. The dimension of the specimen is described as Type V in this standard:

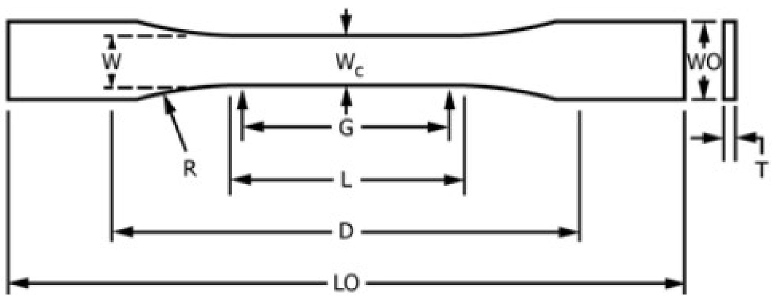


**Figure S2.** Dimensions of tensile testing samples

**Table S1.** Dimensions of tensile testing samples

| **Dimensions (see drawing)** | Specimen dimensions (mm) |
|---|---|
| W—Width of the narrow section | 3.18 |
| L—Length of the narrow section | 9.53 |
| WO—Width overall | 9.53 |
| LO—Length overall | 63.5 |
| G—Gage length | 7.62 |
| D—Distance between grips | 25.4 |
| R—Radius of fillet | 12.7 |

## 3 Curing behavior of modified EP

The DSC curves for all uncured and cured modified EP with 1.5 wt.% modifier concentration are illustrated in **Figure S3**, illustrated complete curing for all modified EP using the given curing conditions in this study.

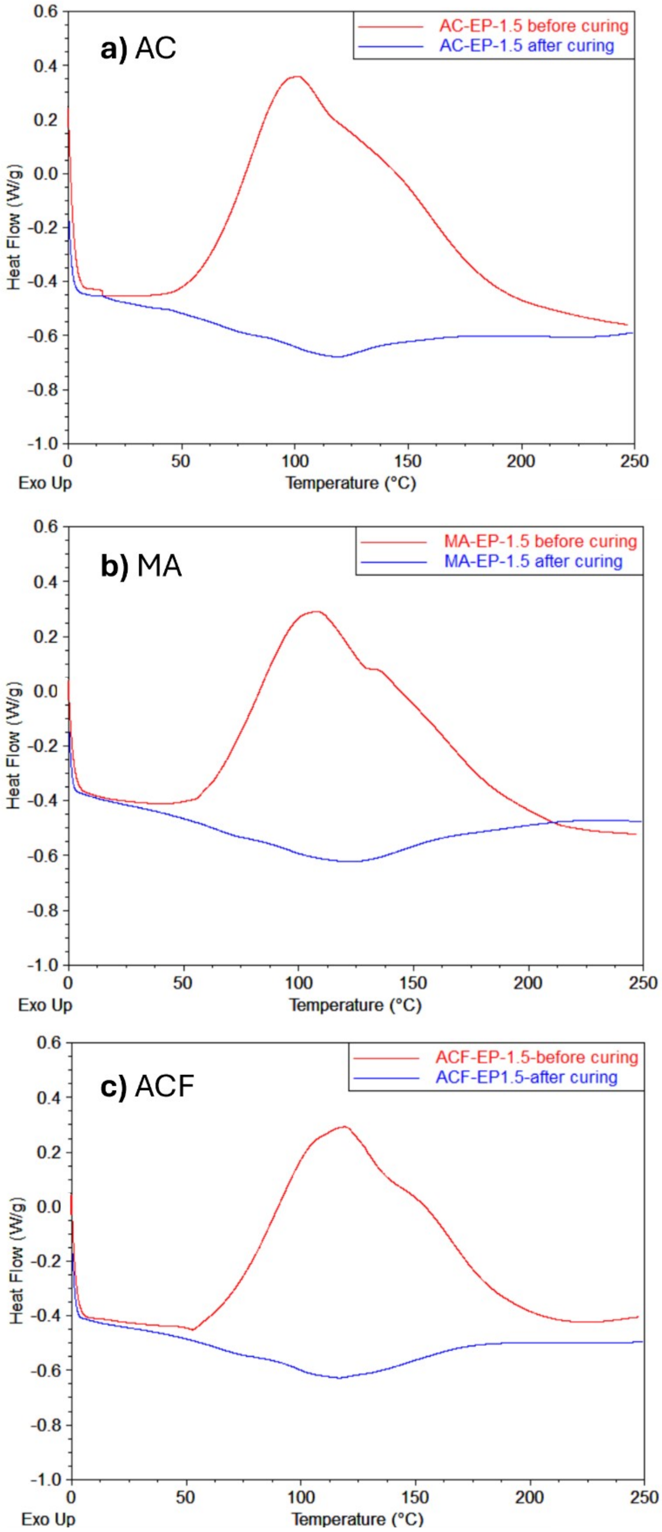


**Figure S3.** DSC curves for uncured and cured **(a)** EP-AC-1.5, **(b)** EP-MA-1.5, and **(c)** EP-ACF-1.5.

## 4 Heat released in curing process of EP-MA

The curing process was investigated by differential scanning calorimetry (DSC). The exothermic peak can be observed in the curing process, as shown in **Figure S4**. As the concentration of MA increases, the heat of curing decreases from 432 J/g (EP-MA-0.5) to 409 J/g (EP-MA-1.0) and to 340 J/g (EP-MA-1.5), indicating reduced crosslinking due to excess modifier.

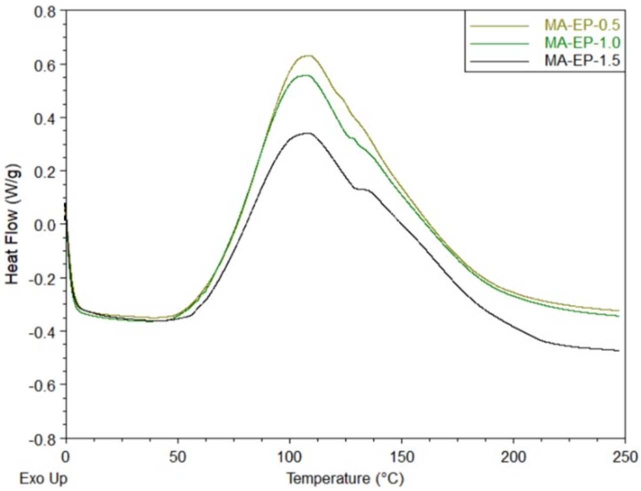


**Figure S4.** Exothermic peaks in curing process for EP-MA with various modifier concentrations.

## 5 First principles calculation for charge trap in EP-MA

First principles calculations indicate that MA introduces deep hole traps at 1.3 eV in the modified EP, as illustrated in **Figure S5**.

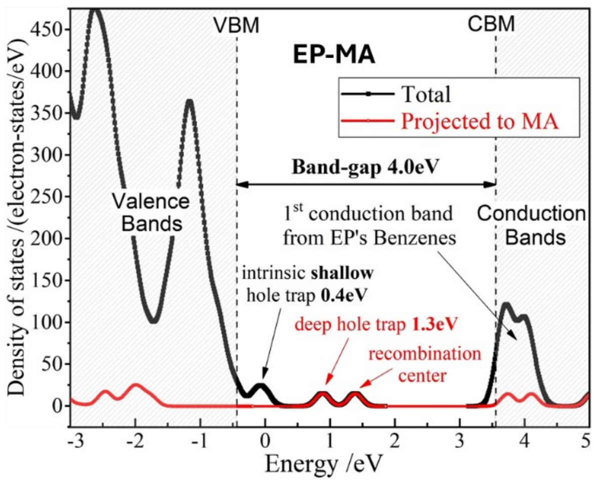


**Figure S5.** Density of electron states for EP-MA calculated through first-principal.

**Reference**


1 R. Ramsdale-Capper and J. P. Foreman, *Polymer*, 2018, **146**, 321–330.
2 J. P. Bell, *Journal of Polymer Science Part A-2: Polymer Physics*, 1970, **8**, 417–436.
3 D20 Committee, *Test Method for Tensile Properties of Plastics*, ASTM International.