Quantum Chemical Study of the Influence of the Catalytic Impurity molecules on the Epoxy-Amine Curing Reaction

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Carbon fiber-reinforced plastics (CFRPs) are used in many fields because of their excellent strength and rigidity while being lightweight. Epoxy resin is a commonly used matrix in CFRPs. In order to improve the performance of epoxy resins, we must design efficient epoxy resin reactions. Due to the multiple combinations of the materials, efficient selections of the curing agents and base epoxy resins are still challenging.

Molecular dynamics (MD) simulation is one of the ideal support tools for investigating suitable combinations, but individual reaction processes that have to be included to treat various combinations are not considered. For that, quantum chemistry (QC) calculations are an excellent way to investigate the reaction process. The properties of individual reactions obtained by the QC calculation can be used for the MD simulation, enabling parameter-free prediction of material characteristics.[1]

In this study, we use a combination of *ab initio* molecular-orbital calculation and the global reaction route map (GRRM) algorithm[2] to determine the transition state structure and obtain the energy of the epoxy-amine curing reaction. This research mainly includes three parts:

1. We have used bisphenol A diglycidyl ether (DGEBA) as the epoxy resin and calculated the reaction paths and activation energies of curing reactions of the DGEBA with four different curing agents (One of the reactions shown in the figure 1).

2. We have simulated reactions under different reaction paths and transition state structures to expand the reaction mechanism at the molecular level. We find a transition state structure of which activation energy is definitely low.

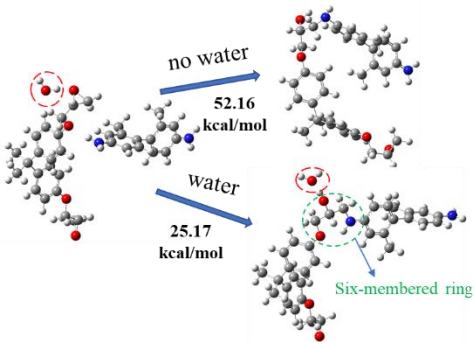

Fig.1: Activation energy under the two reaction paths of DGEBA.

3. Hydroxyl groups or catalytic impurities can catalyze the epoxy-amine curing reaction.[3] For further research on the catalyzed impurities, we have investigated the catalytic effects of alcohol and water added as impurities into the system for the curing reaction of epoxy resin.

[1] Y. Oya *et al.*, "Molecular dynamics simulation for cross-linking processes and material properties of epoxy resins with the first principle calculation combined with global reaction route mapping algorithms" *Chem. Phys. Lett.*, **762,** 138104 (2021).

[2] S. Maeda, K. Ohno, K. Morokuma,"Systematic exploration of the mechanism of chemical reactions: the global reaction route mapping (GRRM) strategy using the ADDF and AFIR methods" *Phys. Chem. Chem. Phys.*, **15**, 3683-3701 (2013).

[3] J.-E. Ehlers, *et al.*, “Theoretical study on mechanisms of the epoxy-amine curing reaction” *Macromolecules,* **40**, 4370– 4377 (2007).