# Multi-Scale Modelling of Epoxy Resin and Composites: from Curing to Fracture

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Polymer modeling across time and length scales can bridge the gap from molecular considerations to the design of macroscopic components and requires understanding in a broad spectrum of physical and chemical phenomena. Quantum mechanical (QM) calculations provide the basis for the formation of atomistic polymer networks on the nano-scale with respect to thermodynamics. Monitoring dynamic processes along fracture by means of molecular dynamics (MM) enable development of coarse-grained models (CG).

We investigated the epoxy system of bisphenol-F-diglycidyl-ether (BFDGE) and 4,6-diethyl-2-methylbenzene-1,3-diamine (DETDA) regarding the crosslinking reaction, as well as bond dissociation, by development of a reactive Force Field, which facilitates our curing algorithm to reach the experimental crosslinking degree of 99% [1,2]. The resulting, reliable models fulfill bulk, especially the elastic properties, we derived from linear response theory [3]. Furthermore, we studied tensile deformation about inter-molecular reorganization processes along fracture processes and extrapolated occurring stresses to vanishing strain rates, which yielded in accordance with macroscopic specimens [2,3]. We also accomplished the transfer from molecular simulation to constitutive modeling by means of a multi-scale modeling capturing deformation and damage in epoxy resins [4]. Addressing the interplay of composite materials, we studied molecular structuring of epoxy at silica and cellulose interfaces [5] as well as corresponding forces along detaching processes [6]. In conclusion, there is a large body of atomistic-level insights available to provide the needed inputs for a coarse-grained setup. This setup will hence not rely on ad hoc assumptions, but directly feature the beforehand identified properties from QM and MM methods.

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[6] Julian Konrad, and Dirk Zahn. Interfaces in reinforced Epoxy Resins: from molecular Scale Understanding towards mechanical properties. *Submitted,* **2023**.