Impact of Curing dynamics on the Microstructure and Properties of Epoxy Thermosets

Sampanna Pahi[1], Christian Wick[1], and Ana-Sunčana Smith[1,2]

[1]PULS Group, Institute for Theoretical Physics, IZNF, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Group of Computational Life Sciences, Ruder Bošković Institute, 10000 Zagreb, Croatia

Epoxy resins, essential in manufacturing, require an understanding of their curing kinetics for optimal properties. This study, using epoxy systems modeled with the recently developed Block Chemistry force-field[1], examines the impact of reaction kinetics on polymer chain formation. We employed a QM/MM methodology to optimize local reaction kinetics at the molecular level, enhancing curing precision. Quantum analyses and simulations showed that secondary reactions prompt early branching, while primary reactions lead to linear growth before crosslinking. Further, incorporating an isomeric mixture in the pre-polymer model resulted in denser packing, mirroring experimental densities. The study also includes loop size distribution analysis within the polymer matrix, crucial for assessing material rigidity and linking microstructural characteristics to macroscopic properties, enriching our understanding of the molecular structure-material behavior relationship in thermoset polymers.

[1] M. Livraghi, S. Pahi, P. Nowakowski, D. Smith, C.R. Wick, A.-S. Smith *The Journal of Physical Chemistry B*, **2023**, *127*, 7648-7662.