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Ab initio molecular dynamics simulations of the thermal degradation of model compounds of industrially-relevant copolyesters EROL YILDIRIM, Fiber and Polymer Science Program, North Carolina State University, ANDREW T. DETWILER, CURT CLEVEN, Eastman Chemical Company, AHMED EL-SHAFEI, MELISSA A. PASQUINELLI, Fiber and Polymer Science Program, North Carolina State University — The thermal degradation of copolyesters can be impacted by a variety of factors beyond the chemical composition of the polymer, including the solvent and processing conditions, as well as the presence of oxygen, moisture, additives, and dyes. Thus, we investigated the role that these factors play for a series of model compounds of industrially relevant copolyesters using ab initio molecular dynamics simulations. The results reveal some interesting trends and correlations to experiments, which can be applied to improve the exterior longevity of copolyesters.

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