Abstract Submitted
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Coarse-grained simulation of polymer-filler blends[1] GREGG LEGTERS, VIKRAM KUPPA, Univ of Dayton, GREGORY BEAUCAGE, Univ of Cincinnati, UNIV OF DAYTON COLLABORATION, UNIV OF CINCINNATI COLLABORATION — The practical use of polymers often relies on additives that improve the property of the mixture. Examples of such complex blends include tires, pigments, blowing agents and other reactive additives in thermoplastics, and recycled polymers. Such systems usually exhibit a complex partitioning of the components. Most prior work has either focused on fine-grained details such as molecular modeling of chains at interfaces, or on coarse, heuristic, trial-and-error approaches to compounding (eg: tire industry). Thus, there is a significant gap in our understanding of how complex hierarchical structure (across several decades in length) develops in these multicomponent systems. This research employs dissipative particle thermodynamics in conjunction with a pseudo-thermodynamic parameter derived from scattering experiments to represent polymer-filler interactions. DPD simulations will probe how filler dispersion and hierarchical morphology develops in these complex blends, and are validated against experimental (scattering) data. The outcome of our approach is a practical solution to compounding issues, based on a mutually validating experimental and simulation methodology.

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