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Sequence-Specific Copolymer Compatibilizers designed via a Genetic Algorithm[1] VENKATESH MEENAKSHISUNDARAM, TARAK PATRA, JUI-HSIANG HUNG, DAVID SIMMONS, Univ of Akron — For several decades, block copolymers have been employed as surfactants to reduce interfacial energy for applications from emulsification to surface adhesion. While the simplest approach employs symmetric diblocks, studies have examined asymmetric diblocks, multiblock copolymers, gradient copolymers, and copolymer-grafted nanoparticles. However, there exists no established approach to determining the optimal copolymer compatibilizer sequence for a given application. Here we employ molecular dynamics simulations within a genetic algorithm to identify copolymer surfactant sequences yielding maximum reductions the interfacial energy of model immiscible polymers. The optimal copolymer sequence depends significantly on surfactant concentration. Most surprisingly, at high surface concentrations, where the surfactant achieves the greatest interfacial energy reduction, specific non-periodic sequences are found to significantly outperform any regularly blocky sequence. This emergence of polymer sequence-specificity within a non-sequenced environment adds to a recent body of work suggesting that specific sequence may have the potential to play a greater role in polymer properties than previously understood.

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