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Determination of Globally Stable Block Copolymer Phases Using Particle Swarm Optimization CAROL TSAI, KRIS DELANEY, GLENN FREDRICKSON, Univ of California - Santa Barbara — The unguided search for the stable phase of a block copolymer of a given composition and architecture is a problem of global optimization with important ramifications from a materials design perspective. A diverse collection of heuristic algorithms for solving global optimization problems is available to employ. In this talk, we discuss the development of a reciprocal-space Particle Swarm Optimization (PSO)-SCFT method applied to a diblock copolymer. By manipulating the Fourier components of SCFT fields near the principal shell, the dimensionality of the search space is greatly reduced compared to algorithms which work directly on the real-space field values.

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