Abstract Submitted for the MAR16 Meeting of The American Physical Society

Unguided discovery of BCP self-assembly: challenges and outlook CAROL TSAI, KRIS DELANEY, GLENN FREDRICKSON, University of California, Santa Barbara — The unguided search for the stable phases of a block copolymer of a given composition and architecture is a problem of global optimization. The appeal of this pursuit arises from both a materials design perspective and also from the perspective of solving global optimization problems via heuristic algorithms. A diverse collection of such algorithms is available to employ, including evolutionary and swarm strategies. In this talk we discuss the development, successes, and challenges of a real-space genetic algorithm (GA)-SCFT method as applied to a diblock copolymer. We then consider alternative representations and algorithms for solving the forward problem in bulk block copolymer systems.

Carol Tsai University of California, Santa Barbara

Date submitted: 02 Nov 2015 Electronic form version 1.4