David Shirokoff* (david.g.shirokoff@njit.edu) and Mahdi Bandegi. Conic programming of a variational inequality for self-assembly.

We examine the problem of minimizing a class of non-local, non-convex functionals, that arise from large systems of pairwise interacting particles. Although finding and verifying local minima to these functionals is relatively straightforward, computing and verifying global minima is much more difficult. Global minima are important as they characterize the most likely observable states for the associated particle systems (interacting in the presence of thermal noise). We discuss how minimizing the energy functionals can be viewed as testing whether an associated bilinear form is co-positive. We then examine sufficient conditions for global optimality obtained through a convex relaxation of the cone of co-positive functionals. The sufficient conditions are (i) often sharp; and (ii) provide an optimal decomposition of the functional (into the sum of a convex and non-negative functional) that can be used to characterize the emerging shapes of self-assembled structures. (Received February 19, 2018)