A new method for developing design strategies for patchy particle self-assembly

Eric Jankowski and Sharon C. Glotzer
Department of Chemical Engineering
University of Michigan

In this work we investigate the structures that can be self-assembled by a family of complex, anisotropic patchy particles. We develop a new method, bottom-up building block assembly, which generates energy-minimizing configurations of these particles more efficiently than thermodynamics based simulation methods. By comparing the energy-minimizing configurations with those that can be self-assembled we introduce the concept of self-assembly propensity and show that it depends upon the assembly pathways available to the building blocks. By grouping generated configurations into motifs we discern important assembly characteristics for specific patterns and identify building blocks with a propensity to self-assemble a desired configuration.