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Computer simulation study on the self-assembly structure of soft Janus particles ZHAO-YAN SUN, ZHAN-WEI LI, Stete Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, MULTI-SCALE SIMULATION TEAM — Soft and deformable Janus particles have received more attention due to their unique properties and enormous potential applications in recent years. Here we present a mesoscale model for soft Janus particles, which successfully reflects their physical nature by directly mapping onto experimentally measurable particle properties. By properly tuning Janus balance and the strength of attraction between attractive patches, soft Janus particles can reversibly self-assemble into a number of fascinating hierarchical superstructures in dilute solutions, such as micelles, wormlike strings, single helices, double helices, bilayers, tetragonal bilayers, complex supermicelles, and in bulk systems, such as the hexagonal columnar structure and the body-centered tetragonal structure. We also introduce a new concept in achieving template-free fabrication of diverse 2D ordered nanostructures by utilizing anisotropic characteristics of soft triblock Janus particles. Our work demonstrates that soft Janus particles with the deformable and non-centrosymmetric characteristics hide many surprises in the design and fabrication of hierarchically self-assembled superstructures.

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