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Engineering Entropy for Colloidal Design YINA GENG, GREG VAN ANDERS, PAUL M. DODD, SHARON C. GLOTZER, University of Michigan, GLOTZER GROUP COLLABORATION — The inverse design of target material structures is a fundamental challenge. Here, we demonstrate the direct inverse design of soft materials for target crystal structures using entropy alone. Our approach does not require any geometric ansatz. Instead, it efficiently samples 92- or 188-dimensional building-block parameter spaces to determine thermodynamically optimal shapes. We present detailed data for optimal particle characteristics and parameter tolerances for six target structures. Our results demonstrate a general, rational, and precise method for engineering new colloidal materials, and will guide nanoparticle synthesis to realize these materials.

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