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Efficient Parameter Searches for Colloidal Materials Design with Digital Alchemy PAUL M. DODD, Department of Chemical Engineering, University of Michigan, Ann Arbor, YINA GENG, Department of Physics, University of Michigan, Ann Arbor, GREG VAN ANDERS, SHARON C. GLOTZER, Department of Chemical Engineering, University of Michigan, Ann Arbor — Optimal colloidal materials design is challenging, even for high-throughput or genomic approaches, because the design space provided by modern colloid synthesis techniques can easily have dozens of dimensions. In this talk we present the methodology of an inverse approach we term "digital alchemy" to perform rapid searches of design-paramenter spaces with up to 188 dimensions that yield thermodynamically optimal colloid parameters for target crystal structures with up to 20 particles in a unit cell. The method relies only on fundamental principles of statistical mechanics and Metropolis Monte Carlo techniques, and yields particle attribute tolerances via analogues of familiar stress-strain relationships.

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