## Abstract Submitted for the MAR16 Meeting of The American Physical Society

Digital Alchemy for Materials Design: Colloids and Beyond GREG VAN ANDERS, DAPHNE KLOTSA, ANDREW KARAS, PAUL DODD, SHARON GLOTZER, University of Michigan — Starting with the early alchemists, a holy grail of science has been to make desired materials by manipulating basic building blocks. Building blocks that show promise for assembling new complex materials can be synthesized at the nanoscale with attributes that would astonish the ancient alchemists in their versatility. However, this versatility means that connecting building-block attributes to bulk structure is both necessary for rationally engineering materials and difficult because building block attributes can be altered in many ways. We show how to exploit the malleability of colloidal nanoparticle elements to quantitatively link building-block attributes to bulk structure through a statistical thermodynamic framework we term digital alchemy. We use this framework to optimize building blocks for a given target structure and to determine which building-block attributes are most important to control for self-assembly, through a set of novel thermodynamic response functions. We thereby establish direct links between the attributes of colloidal building blocks and the bulk structures they form. Moreover, our results give concrete solutions to the more general conceptual challenge of optimizing emergent behaviors in nature and can be applied to other types of matter.

> Greg van Anders University of Michigan

Date submitted: 06 Nov 2015 Electronic form version 1.4