Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Shaping Crystal-Crystal Phase Transitions XIYU DU, GREG VAN ANDERS, JULIA DSHEMUCHADSE , SHARON GLOTZER, Univ of Michigan - Ann Arbor — Previous computational and experimental studies have shown self-assembled structure depends strongly on building block shape. New synthesis techniques have led to building blocks with reconfigurable shape and it has been demonstrated that building block reconfiguration can induce bulk structural reconfiguration. However, we do not understand systematically how this transition happens as a function of building block shape. Using a recently developed digital alchemy[1] framework, we study the thermodynamics of shape-driven crystal-crystal transitions. We find examples of shape-driven bulk reconfiguration that are accompanied by first-order phase transitions, and bulk reconfiguration that occurs without any thermodynamic phase transition. Our results suggest that for well-chosen shapes and structures, there exist facile means of bulk reconfiguration, and that shape-driven bulk reconfiguration provides a viable mechanism for developing functional materials. [1] G. van Anders, D. Klotsa, A. S Karas, P. M Dodd, and S. C Glotzer, ACS Nano, 9, 9542 (2015).

Xiyu Du
Univ of Michigan - Ann Arbor

Date submitted: 06 Nov 2015 Electronic form version 1.4