Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Modeling two-dimensional materials self-assembly: from Honeycomb to Kagome lattices SIMISO K. MKHONTA, Wayne State University, KEN R. ELDER, Oakland University, ZHI-FENG HUANG, Wayne State University — Novel two-dimensional materials of graphene-type and beyond have been of great interest in both fundamental research and a wide range of applications. In this work we study the self assembly properties of these 2D structures via the development of a phase-field-crystal model. The free energy functional in the model is designed to favor self assembly in crystals commensurate with a triangular symmetry, leading to a range of complex phases including honeycomb, kagome, and oblique, in addition to the simple triangular phase. We also examine the elastic properties of these novel crystalline structures, and the nonequilibrium evolution processes of these systems which are governed by diffusive time-scale dynamics.

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Date submitted: 08 Nov 2012 Electronic form version 1.4