

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Experiment-scale molecular simulation study of liquid crystal thin films** TRUNG DAC NGUYEN, JAN-MICHAEL Y. CARRILLO, MICHAEL A. MATHESON, W. MICHAEL BROWN, National Center for Computational Sciences, Oak Ridge National Laboratory — Supercomputers have now reached a performance level adequate for studying thin films with molecular detail at the relevant scales. By exploiting the power of GPU accelerators on Titan, we have been able to perform simulations of characteristic liquid crystal films that provide remarkable qualitative agreement with experimental images. We have demonstrated that key features of spinodal instability can only be observed with sufficiently large system sizes, which were not accessible with previous simulation studies. Our study emphasizes the capability and significance of petascale simulations in providing molecular-level insights in thin film systems as well as other interfacial phenomena.

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Date submitted: 14 Nov 2013

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