Abstract Submitted
for the OSF11 Meeting of
The American Physical Society

Complete Phase Diagram of a Single Polymer Chain[1] MARK TAYLOR, Dept. of Physics, Hiram College, WOLFGANG PAUL, Martin-Luther-Universitat, Halle, Germany, KURT BINDER, Johannes-Gutenberg-Universitat, Mainz, Germany — The phase behavior of a single homopolymer chain is analogous to that of simple liquid, exhibiting an expanded coil (gas-like) phase, a collapsed globule (liquid-like) phase, and a compact solid phase. Using Wang-Landau sampling with bond-rebridging Monte Carlo moves we have studied the complete phase behavior of a flexible interaction-site polymer chain comprised of up to 256 square-well-spheres [1]. Here we present a finite-size scaling analysis for the phase behavior of a SW chain in the long chain limit. For a sufficiently short interaction range, the chain undergoes a direct freezing transition from the expanded coil without an intervening collapse transition. These results confirm the recent lattice model prediction that a collapsed-globule state is unstable with respect to a solid phase for polymers with sufficiently short-range monomer-monomer interactions [2].

[1] M.P. Taylor, W. Paul, and K. Binder, J. Chem. Phys. 131, 114907 (2009).
[2] W. Paul, T. Strauch, F. Rampf, and K. Binder, Phys. Rev. E 75, 060801(R) (2007).

[1]Funding: NSF DMR-0804370, DFG SFB-625/A3

Mark Taylor
Dept. of Physics, Hiram College

Date submitted: 09 Sep 2011 Electronic form version 1.4