

Abstract Submitted
for the MAS14 Meeting of
The American Physical Society

Phase Transitions in a Model of Y-Shaped Molecules¹ DONOVAN RUTH, Lehigh University, RAUL TORAL, University of Balearics Islands, DANIELLE HOLZ, Drew University, JAMES GUNTON, Lehigh University — Increasing attention in statistical mechanics is being given to non-spherical molecules, such as polypeptide chains and protein molecules. One example is provided by immunoglobulin, which has a “Y” shape. In this work, we determine the phase diagram of “Y”-shaped molecules on a triangular lattice through Monte Carlo Grand Canonical ensemble simulation, using histogram reweighting and multicanonical sampling. We show that this system is a member of the Ising universality class through finite size scaling techniques. The molecules interact via the distal tips with the nearest neighbor distal ends of other molecules; There are no center to center interactions, center to tip, or molecule to lattice interactions included in this particular study. For low temperatures, multicanonical sampling was implemented to induce faster phase transitions in the simulation. Studying several system sizes, finite size scaling was used to determine the two phase coexistence curve, bulk critical temperature, and critical chemical potential.

¹This work is funded by the G. Harold and Leila Y. Mathers Foundation.

Donovan Ruth
Lehigh University

Date submitted: 29 Aug 2014

Electronic form version 1.4