

Abstract Submitted  
for the MAR16 Meeting of  
The American Physical Society

**The effects of bonded interactions on the structural phase properties of flexible elastic homopolymer** KAI QI, BENJAMIN LIEWEHR, TOMAS KOCI, BUSARA PATTANASIRI, MATTHEW WILLIAMS, MICHAEL BACHMANN, The Univ of Georgia — By means of advanced parallel-tempering replica-exchange Monte Carlo methods we systematically examine the effects of an asymmetric bond potential between the bonded monomers on the structural formations of an elastic flexible polymer model. Employing microcanonical inflection-point analysis and conformational analysis based on a suitable set of structural order parameters, we identify diverse structural phases in the low-temperature region of the microcanonical hyperphase diagram. In addition to the icosahedral phase occurring if the symmetry of the bonded interaction is broken by strong bonded Lennard-Jones potential, amorphous structures with bihexagonal cores appear for small values of the asymmetry control parameter in the bond potential. Another remarkable feature is the observation of the hierarchy of freezing transitions associated with the formation of the surface layer after nucleation.

Kai Qi  
The Univ of Georgia

Date submitted: 06 Nov 2015

Electronic form version 1.4