

Abstract Submitted  
for the MAR05 Meeting of  
The American Physical Society

Sorting Category: 04.14 (C)

**Monte Carlo study of reversibly associated polymers<sup>1</sup>**

CHUN-CHUNG CHEN, ELENA E. DORMIDONTOVA, Department of Macromolecular Science and Engineering, Case Western Reserve University, Cleveland, Ohio 44106 — Monte Carlo simulations are applied to study polymers formed through reversible associations of end-functionalized oligomers. The associations are either through donor-acceptor-type complementary bonding or through two-to-one ligand-metal complexation. For donor-acceptor-type reversible polymers, we study the effects of oligomer length, bond stiffness and concentration on the degree of association and ring-chain equilibrium. For the metallo-supramolecular polymers, the effects of the energy of complexation, cooperativity of the ligand-metal bonds, and the metal concentration on the degree of association and average molecular weight are considered. Criteria for obtaining high molecular weight polymers in a broad range of metal concentrations are suggested based on the simulation and analytical results.

<sup>1</sup>This work was supported by the National Science Foundation under CAREER Award CHE-0348302.

Prefer Oral Session  
 Prefer Poster Session

Chun-Chung Chen  
chun-chung.chen@case.edu  
Case Western Reserve University

Date submitted: 30 Nov 2004

Electronic form version 1.4