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Monte Carlo study of reversibly associated polymers[1] 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.

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Chun-Chung Chen
Case Western Reserve University

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