Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Computer Simulation of a Switchable Metallo-Supramolecular Gel[1] SHIHU WANG, ELENA DORMIDONTOVA, Department of Macromolecular Science and Engineering, Case Western Reserve University — Using Monte Carlo simulation, we studied reversible metallo- supramolecular gel comprised of linear oligomers end- functionalized with ligands and metal ions that can form trans- or cis- ligand-metal complexes with a ratio up to 3:1. We found that cis- isomers exhibit a larger overall degree of association and higher average molecular weight compared to trans- isomers due to a larger fraction of 3:1 or 2:1 ligand- metal complexes. Furthermore the metallo-supramolecular gel formed by cis-isomers occurs within a wider range of metal-to- oligomer ratios at a lower oligomer concentration and exhibits a larger elastic modulus and a smaller mesh-size compared to gel formed by trans-isomers. We found that exchanging cis- to trans- isomers leads to a monotonic change of the materials properties for most cases except for the 2:1 ligand:metal ratio at which the mesh size exhibits a minimum due to the favorable formation of intramolecular bonds by cis- isomers. These switchable properties suggest interesting application opportunities.

[1]This work was supported by the NSF Career Award CHE-0348302.

Elena Dormidontova
Department of Macromolecular Science and Engineering,
Case Western Reserve University

Date submitted: 11 Dec 2008 Electronic form version 1.4