Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Self-Consistent Field Modeling of Diblock Copolymers in Selective Solvents[1] RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN 55455 — The purpose of my poster is to study the driving forces behind the self-assembly of a diblock copolymer AB, consisting of a solventphilic block (B) and a solventphobic block (A), in selective solvents (S). Micellar transformations between spherical, cylindrical, and bilayer curvatures for a model system are tracked using self-consistent field modeling, in real space, in the dilute regime. The transition from a concentrated regime, $\phi_{\mathrm{AB}} \sim 1$, to a dilute regime, $\phi_{\mathrm{AB}} \sim 0$, is studied. Phase portrait for the concentrated regime is generated using periodic self-consistent field modeling. The unbinding transition, as seen in the periodic counterpart of self-consistent field theory, is compared with the transformations observed in the dilute regime. The two phase regions in the dilute regime are mapped out for the inverted phases as well.

[1]This work was supported by UMN MRSEC (support for Raghuram Thiagarajan) using computer resources provided by both the Minnesota Supercomputing Institute and the UMN MRSEC.

Raghuram Thiagarajan
Department of Chemical Engineering and Materials Science,
University of Minnesota, Minneapolis, MN 55455

Date submitted: 20 Dec 2010 Electronic form version 1.4