Abstract Submitted for the MAR12 Meeting of The American Physical Society

Modeling of Interactions Between Spherical Micelles for Diblock Copolymers in Selective Solvents RAGHURAM THIAGARAJAN, DAVID MORSE, Department of Chemical Engineering and Materials Science, University of Minnesota — The self-assembly of spherical micelles formed in systems with a diblock copolymer AB, consisting of a solvent-philic block (B) and a solvent-phobic block (A), in selective solvents (S) is studied here. Effective interactions between spherical micelles for a model system are quantified using self-consistent field modeling in real space, for the dilute regime $\phi_{AB} < 0.2$, as well as using a pseudo-spectral implementation of SCFT, for the concentrated regime $\phi_{AB} > 0.2$. We show that the free energy of BCC, and FCC phases can be described in terms of a single effective pair potential that depends on micelle aggregation number, but the aggregation number changes significantly with concentration as well as temperature.

> Raghuram Thiagarajan Dept of Chemical Engineering and Materials Science, University of Minnesota

> > Electronic form version 1.4

Date submitted: 14 Nov 2011