Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Micellization behavior of Poly[2,7-(9,9-dihexylfluorene)]-*b*-Poly(2-vinylpyridine) in MeOH/THF Mixed Solvents via a Combination of Coarse-Grained and All-Atom Molecular Dynamics Methods[1] CHIN-WEN CHEN, JING-SAIN LIN, WEN-CHANG CHEN, CHING-I HUANG, National Taiwan University, CHEN WEN-CHANG COLLABORATION — Coarse-grained (CG) and all-atom (AA) molecular dynamics (MD) methods are proposed to investigate the micellar behavior of a semiconducting conjugated diblock polymer, poly[2,7-(9,9-dihexylfluorene)]-*b*-poly(2-vinylpyridine) (PF-*b*-P2VP) in MeOH/THF. We adopt the iterative Boltzmann inversion method to obtain CG force filed through mapping route with AA MD data. In order to compare experimental result [1], we first choose PF_8-*b*-$P2VP_{11}$ with Φ =0.1 and varying ratio of MeOH/THF. When MeOH/THF = 0/100, due to the fact the THF is a common solvent. We observe no micellar formation with increasing ratio of P2VP selective solvent in MeOH/THF from 0/100 to 30/70. The PF block tends to aggregate to form micelles, and size of micelle keeps increasing. The spherical micelles transform into the worm-like formation in 90/10. Our simulation results are in agreement with the experimental study, indicating the constructive CGMD parameters are successful to describe the PF-*b*-P2VP in MeOH/THF.

[1] *Macromolecules*, **41**, 8759-8769 (2008)

[1]Financial support from National Science Council of Taiwan (NSC-99-2120-M-002-009). Prof. Monica Olvera de la Cruz, Dr. Rastko Sknepnek and Ms. Ting I.N.G. Li, Northwestern University.

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Date submitted: 08 Jan 2013 Electronic form version 1.4