Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Multi scale computer simulations of the self-assembly of block copolymeric beta-peptides JAGANNATH MONDAL, ARUN YETHIRAJ, University of Wisconsin Madison — There is considerable interest in a class of molecules made from β-amino acids (which contain an additional backbone carbon atom when compared with natural amino acids). Block copolymers of β-peptides, where one block is hydrophobic and the other is hydrophilic, self-assemble into micelles. In this work we use computer simulations to provide insight into the self-assembly of these molecules. All-atom simulation results for the free energy of association of a pair of these block co polymeric β- peptides show that a *homochiral* hydrophobic block promotes self assembly compared to a *heterochiral* hydrophobic block, consistent with experiment. We have also developed a coarse-grained model for these block copolymers and simulations using this model show that these molecules spontaneously forms micelles, and the morphology of these micelles is concentration dependent, with spherical micelles at low concentrations and worm-like micelles at high concentrations.

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Date submitted: 16 Nov 2010 Electronic form version 1.4