Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Multi-scale morphology in self-assembly of peptides to proteins via a coarse-grain model[1] RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Self-organizing structures of short peptides (6-7 residues) and proteins (136 residues) are studied by a coarse-grained Monte Carlo simulation. Peptides and proteins are described by coarse-grained chains of residues whose interactions are described by a knowledge-based residue-residue interaction potential that captures the compositional specificity. Large-scale computer simulations are performed to study the structural evolution e.g. aggregation, network, etc. at a range of temperatures and concentrations. A number of local and global physical quantities including structure factor are examined. We find that the residue interactions, concentration, and size of chains are very important in modulating the structure of emerging morphologies in the specified temperature range. Estimates are provided for the effective (fractal) dimension of the assembly over various length scales as a function of temperature.

[1]This work is supported by the Air Force Research Laboratory.

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Date submitted: 03 Nov 2014 Electronic form version 1.4