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Scaffolding of peptides using a coarse-grained representation of residues with side chain and backbone nodes[1] RAS PANDEY, University of Southern Mississippi, BARRY FARMER, Air Force Research Laboratory — Monte Carlo simulations are performed to study scaffolding of peptides (KSL) on a cubic lattice. A residue is represented by three backbone nodes (C-terminal, C-alpha, N-terminal) and a side node connected to the central C-alpha node each connected by fluctuating bond. A peptide is a chain of residues. A solvent constituent is represented by a particle of the same size as that of a node. Peptides and solvent are distributed randomly in the cubic box with concentration C_p and C_w respectively. Each residue interacts with other residues and solvent particles via its side chain with the Lennard-Jones (LJ) potential where a knowledge-based interaction matrix is used for the residue-residue interaction. We examine local and global physical quantities such as mobility and energy of each residue, radial distribution function, and structure factor. We find that the scaffolding of peptides depends on the interaction strength and concentration of the solvent. The structure factor shows multi-scale structure of the aggregates.

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