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Micro-phase assembly of active sites in a coarse-grained model of chromatin by Monte Carlo simulation[1] YANG ZHANG, DIETER HEERMANN, University of Heidelberg, Germany, BARRY FARMER, Air Force Research Laboratory, RAS PANDEY, University of Southern Mississippi — A coarse-grained model is used to study the self-assembly of active sites in a DNA (chromatin) chain. The chromosome is described by a bond-fluctuating chain of two types of nodes A (interacting) and B (non-interacting), distributed randomly with concentration C and $1-C$ respectively. Active nodes interact with a Lennard-Jones (LJ) potential and execute their stochastic motion with the Metropolis algorithm. The depth of the LJ potential (f), a measure of interaction strength and the concentration (C) of the active sites are varied. A number of local and global physical quantities are studied such as mobility (M_n) profile of each node, their local structural profile, root mean square (RMS) displacement (R), radius of gyration (R_g), and structure factor $S(q)$. We find that the chain segments assemble into microphase of blobs which requires higher concentration of active sites at weaker interaction. These findings are consistent with that of a dynamic loop model of chromatin on global (large) scale but differ at small scales.

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