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Conformation and Dynamics of a Flexible Sheet in Solvent Media by Monte Carlo Simulations RAS PANDEY, University of Southern Mississippi, KELLY ANDERSON, Air Force Research Laboratory, HENDRIK HEINZ, Wright State University, BARRY FARMER, Air Force Research Laboratory — Flexibility of the clay sheet is limited even in the ex-foliated state in some solvent media. A coarse grained model is used to investigate dynamics and conformation of a flexible sheet to model such a clay platelet in an effective solvent medium on a cubic lattice of size L^3 with lattice constant a. The undeformed sheet is described by a square lattice of size L_s^2, where, each node of the sheet is represented by the unit cube of the cubic lattice and $2a$ is the minimum distance between the nearest neighbor nodes to incorporate the excluded volume constraints. Additionally, each node interacts with neighboring nodes and solvent (empty) sites within a range r_i. Each node execute their stochastic motion with the Metropolis algorithm subject to bond length fluctuation and excluded volume constraints. Mean square displacements of the center node and that of its center of mass are investigated as a function of time step for a set of these parameters. The radius of gyration (R_g) is also examined concurrently to understand its relaxation. Multi-scale segmental dynamics of the sheet is studied by identifying the power-law dependence in various time regimes. Relaxation of R_g and its dependence of temperature are planned to be discussed.

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