Abstract Submitted
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Clay platelets in a matrix of amino acids (of a clay binding peptide M1) homopolymer: binding, unbinding, dispersion, and self-assembly by a coarse-grained Monte Carlo simulation[1] BARRY FARMER, LAWRENCE DRUMMY, SHARON JONES, RICHARD VAIA, RAJESH NAIK, Air Force Research Laboratory, HENDRIK HEINZ, University of Akron, RAS PANDEY, University of Southern Mississippi — Monte Carlo simulations are performed to study binding and distribution of a stack of clay platelets in a matrix of homo-polymers of residues. The set of residue monomers is selected from a clay binding peptide $(M1)$[1]. The length of homopolymer is same as that the peptide $M1$. Clay platelet and amino acid polymer (AAP) are described by a bond-fluctuation model[2] where specificity of each residue interaction is incorporated. Each node (of clay platelets and AAP) performs their stochastic motion via Metropolis algorithm subject to steric and excluded volume constraints. We examine the mobility of AAP and platelets and their density profiles. We find that dispersion and binding of each AAP is unique and differ from that of the clay platelets in peptide $M1$ matrix.

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