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Probability of adsorption of peptide (CR3-1, S2) chains on clay minerals by coarse-grained Monte Carlo simulation RAS B. PANDEY, University of Southern Mississippi, HENDRIK HEINZ, University of Akron, BARRY L. FARMER, SHARON JONES, LAWRENCE F. DRUMMY, RAJESH R. NAIK, Air Force Research Laboratory, WPAFB — A coarse-grained description is used to study the structure and dynamics of peptide chains (CR3-1, S2) in presence of a clay surface on a cubic lattice. A peptide chain is represented by the specific sequence of amino acids. Specificity of residues is captured via an interaction matrix based on the insight gained from the atomistic simulation, i.e., each residue interacts with surrounding residues, solvent, and the clay surface with a unique interaction potential. We use a standard LJ potential with its coefficient controlled by the interaction matrix. Simulations are performed with a number of peptide chains. Along with the global energy and dynamics of peptides, we keep track of mobility, energy (total and adsorption), and correlation with the local structure from the density profiles of each residue. Based on the analysis of local and global quantities, we are able to assess the probability of adsorption of peptides to clay surface in agreement with experiment. The probability of adsorption of S2 is found to be much higher than that of CR3-1 in which S2 is anchored by Lysine. The procedure is complementary to biopanning experiments since it allows screening a large number of peptides (more than 10E+5) on the surface to estimate their binding potential.

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