

Abstract Submitted  
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**Binding of peptides (CR3-1, S2) to clay substrate and their intercalation in clay galleries by a coarse-grained Monte Carlo simulation<sup>1</sup>**

LAWRENCE DRUMMY, SHARON JONES, BARRY FARMER, 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 of peptides (CR3-1: *Trp-Pro-Ser-Ser-Tyr-Leu-Ser-Pro-Lle-Pro-Tyr-Ser* and S2: *His-Gly-Lle-Asn-Thr-Thr-Lys-Pro-Phe-Lys-ser-Val*) to a clay substrate and a stack of mobile platelets on a cubic lattice. A bond-fluctuation description is used to model both clay platelet and the peptide chains. Specificity of each residue is incorporated via an interaction matrix for the residue–residue and residue-clay interactions guided by an all-atom MD simulations and their hydrophobicity. We examine the mobility of each residue, the energy, and their density profiles, and correlation profiling the proximity to the substrate or a stack of mobile platelets. The exfoliation and dispersion of the platelets are analyzed as a function of peptide concentration. The interstitial spacing between the platelets, i.e., the average height of the gallery is found to increase due to binding of S2 and its intercalation, consistent with the laboratory observations.

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