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Immobilization dynamics of a tethered membrane by peptide binding - a coarse-grained computer simulation model[1] RAS PANDEY, University of Southern Mississippi, HENDRIK HEINZ, University of Akron, BARRY FARMER, Air Force Research Laboratory — A coarse-grained description is used to model a tethered membrane (also a representation of a clay platelet) immersed in peptide solutions (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*) on a cubic lattice. Using all-atom simulations, X-ray crystallographic data, and the hydrophobicity of each residue as input, an interaction matrix is developed for residue–residue and residue-clay interactions. Dynamics of the membrane and CR3-1 or S2 peptides is examined as a function of peptide concentration among other quantities such as density profiles, binding energy of each residue, mobility and their proximity profile around the membrane. Simulations show that S2 binds to the membrane anchored by Lysine interactions while CR3-1 does not. Binding of S2 slows down the membrane, leading to its pinning. How fast the immobilization of the membrane occurs depends on the peptide concentration.

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