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Adsorption-desorption of peptide chains on Au surface by a coarse-grained Monte Carlo simulation RAS B. PANDEY, University of Southern Mississippi, HENDRIK HEINZ, University of Akron, LAWRENCE R. DRUMMY, RICHARD A. VAIA, RAJESH R. NAIK, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Using a coarse grained description, we study stability of the structure and dynamics of several peptide chains (A3, Flg, Pro10, Gly10, Pd2, Pd4) at gold surfaces on a cubic lattice. Although the structural details within the amino acid groups are ignored, the specificity of their interactions is incorporated in our computer simulation modeling of these peptide chains on a cubic lattice. Appropriate coarse-grained interactions (Lennard-Jones) among the amino acid nodes, solvent, and the gold surface with different strength are guided by the atomistic simulations and X-ray crystallographic data; the molecular weight of each amino acid groups is also considered. Peptide chains execute their stochastic motion and their proximity to the generic gold surface is monitored. Mobility of each amino acid (node), its energy, and correlations to their neighboring constituents are analyzed. Some of these results are consistent with the atomistic simulation.

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