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**Peptide binding to sheet silicate and metal nanoparticles: Insight from atomistic simulation** HENDRIK HEINZ, University of Akron, RAS B. PANDEY, University of Southern Mississippi, LAWRENCE DRUMMY, RICHARD A. VAIA, RAJESH R. NAIK, BARRY L. FARMER, Air Force Research Laboratory, WPAFB — Short peptides (8 to 12 amino acids, excluding Cys) bind selectively to nanoparticles composed of Au, Pd, and montmorillonite depending on the sequence of amino acids, as evidenced by laboratory screening of several billion peptides. The molecular reasons for binding versus non-binding and the specificity toward a certain surface are analyzed by molecular dynamics simulation, using recent force field extensions for fcc metals and sheet silicates to reproduce surface and interface energies with <10% deviation compared to experiment. Polarization on even metal surfaces ranges from 3 to 5 kcal/mol and non-covalent binding energies from 0 and 80 kcal/mol per dodecapeptide. Adsorption energies, changes in chain conformation, Ramachandran plots, and orientational parameters, are analyzed in conjunction with NMR, TEM, and other experimental data. On montmorillonite, an ion exchange reaction of Lys side groups against alkali ions as well as interactions between alkali cations and polar groups in the peptide are explained.

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