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Simulation of Peptide Binding to Silica and Silica Mineralization

F.S. EMAMI, H. HEINZ, Department of Polymer Engineering, The University of Akron, Akron, Ohio, 44325, USA, R.J. BERRY, V. VARSHNEY, B.L. FARMER, R.R. NAIK, AFRL/RXB, WPAFB, Daton, OH 45433, USA, S.V. PATWARDHAN, C.C. PERRY, Department of Chemistry, Nottingham Trent University, Nottingham, NG11 8NS, U.K. — The purpose of this study is to identify the nature of the interaction of peptides with silica surfaces and their effect on mineralization. Classical force fields (CVFF, PCFF) have been extended for silica aiming at the computation of surface properties in quantitative agreement with experiment, taking explicitly into account water molecules, pH, and surface coverage with peptides. We focus on the interaction of five short peptides (pep1, pep4, 82-4, H4, R5) identified by biopanning with regular and amorphous silica surfaces (Q3 and Q2) to understand the relation between peptide sequence and affinity to the surface. Results of the atomistic molecular dynamics simulation indicate adsorption energies, binding constants and conformational changes upon adsorption. The comparison of NMR chemical shifts in solution and on the surface in computation and experiment further aids in understanding the mechanism of binding.

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