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Characterization of Peptide/Surface Interactions for MoS2, Graphene, and Silica. ANDREW STROUD, Louisiana Tech University , PEDRO DEROSA, Louisiana Tech University, Grambling State University , RAJIV BERRY, GARY LEUTY, AFRL Materials and Manufacturing Directorate, CHRIS MURATORE, University of Dayton — Surface-binding peptides are increasingly being used to functionalize inorganic interfaces for bio sensing and 3D-printed bioengineered applications. In this study, classical molecular dynamics was used to identify the structural characteristics of peptide sequences that selectively mediate the binding of graphene and molybdenum disulfide (MoS2) to glass. These three surfaces were exposed to two peptide sequences in aqueous solution. The binding ability of the polypeptides, HSSYWYAFNNKT (P1) and HLLQPTQNPFRN (HLL), toward each surface was compared by calculating binding enthalpies and tracking the positions of critical amino acid residues during the simulations to determine which residues bonded to each surface. For graphene and MoS2, the strongest-binding residues contained aromatic rings. Notably, these amino acids were found within the bulk water layer above the silica surface. Conversely, charged residues bound to silica did not show strong binding to MoS2 or graphene. The relevance of this finding is that as the list of residues that are found to bind to silica is different from those that bind to MoS2 or graphene, such polypeptides can simultaneously bind to both surfaces, acting as a mediator for the 3D printing of 2D materials on glass.

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