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**Investigating the Binding of Peptides to Graphene Surfaces for Biosensing Applications** AMANDA GARLEY, NABANITA SAIKIA, University of Colorado - Boulder, STEPHEN BARR, GARY LEUTY, RAJIV BERRY, Air Force Research Laboratory, HENDRIK HEINZ, University of Colorado - Boulder — The Air Force Research Lab is focused on developing highly selective and sensitive graphene-based sensors functionalized with peptides for biomolecule detection. To achieve this there is a need to model interfacial binding interactions between the organic and inorganic components to complement ongoing experimental investigations. It is important to characterize the binding behavior of individual amino acids, with the goal of predicting binding of large peptides. Since polarization is important in graphene systems, a new force field which includes polarizability is used. This allows for an in depth exploration of pi-pi interactions, electrostatics and van der Waals forces involved with binding. The binding strength is determined via enthalpy and free energy calculations. Additionally, structural quantities are computed, such as how aromatic rings align with the graphene surface and the arrangement of various residue substituents in relation to the surface and water layers. Computational results are useful in guiding experimental methods focused on rapidly screening optimal peptide sequence for binding.

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