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Computational Modeling Studies of Peptides and Proteins on Inorganic Surfaces

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Biological moieties offer exquisite sensitivity and selectivity in their interactions with small molecules, offering considerable potential in applications as chemical sensors. To detect binding events between the peptide and the intended molecule, a transduction mechanism is needed. This often involves an association of the peptide with an inorganic surface, such as a metal nanoparticle, a carbon nanotube, or graphene. Understanding the nature of the association of the peptide with the surface and its effect on the conformational (and thus, binding) properties of the peptide are key to optimizing the sensing mechanism. We utilized computational approaches ranging from *ab initio* to molecular dynamics to bond-fluctuation Monte Carlo methods to study the adsorption of peptides and proteins on inorganic surfaces to develop an understanding of the role that composition and substrate character plays in the adsorption process, and in turn, the effects on the binding events with the molecules of interest.