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Aqueous amino acids and proteins near solid surfaces: ZnO, ZnS, Au, and mica[1]

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We calculate potentials of the mean force for 20 amino acids in the vicinity of the (111) surface of Au, four surfaces of ZnO, and the (110) surface of ZnS using molecular dynamics simulations combined with the umbrella sampling method. In the case of Au, we compare results obtained within three different force fields: one hydrophobic (for a contaminated surface) and two hydrophilic – with and without polarization of the solid. The properties of water near the surface sensitively depend on the force field. All of these fields lead to good binding with very different specificities and to unlike patterns in the density and polarization of water. We demonstrate that binding energies of dipeptides are distinct from the combined binding energies of their amino acidic components. We show that ZnS is more more hydrophobic than ZnO and that the density profile of water is quite different than that forming near ZnO – it has only a minor articulation into layers. Furthermore, the first layer of water is disordered and mobile. In the case of ZnS, not all amino acids can attach to the surface and when they do, the binding energies are comparable to those found for the surfaces of ZnO (and to hydrogen bonds in proteins) but the nature of the specificity is distinct. The covalent bond with the sulfur atom on cysteine is modeled by the Morse potential. For the hydrophobic Au, adsorption events of a small protein (the tryptophan cage) are driven by attraction to the strongest binding amino acids. This is not so for ZnO, ZnS and for the hydrophilic models of Au – a result of smaller specificities combined with the difficulty for proteins, but sometimes not for single amino acids, to penetrate the first layer of water. Molecular dynamics studies of several proteins near mica with a net charge on its surface indicate existence of two types of states: deformed and unfolded. Using a coarse-grained model, we also study a glassy behavior of protein layers at air-water interfaces. REFERENCES: [1] A. Starzyk and M. Cieplak, Denaturation of proteins near polar surfaces, J. Chem. Phys. 135, 235103 (2011); [2] G. Nawrocki and M. Cieplak, Amino acids and proteins at ZnO-water interfaces in molecular dynamics simulations, Phys. Chem. Chem. Phys. 15, 13628-13636 (2013); [3] G. Nawrocki and M. Cieplak, Interactions of aqueous amino acids and proteins with the (110) surface of ZnS in molecular dynamics simulations, J. Chem. Phys. 140, 095101 (2014); [4] G. Nawrocki and M. Cieplak, Aqueous Amino Acids and Proteins Near the Surface of Gold in Hydrophilic and Hydrophobic Force Fields, J. Phys. Chem. C 118, 12929-12943 (2014); [5] M. Cieplak, D. B. Allen, R. L. Leheny, and D. H. Reich, Proteins at air-water interfaces: a coarse-grained approach, Langmuir (in press).

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