About the interaction of (bio)molecules and materials surfaces in aqueous ionic solutions – an atomistic study

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It is well known that interactions of molecules depend not only on their own architecture. Rather, water which is always present in a biological environment significantly determines the nature of molecular contacts. Especially for molecules or particles with titratable surface groups, additional environmental influences, such as ionic strength or pH thus contribute to the electrostatic distribution of the molecular surfaces and determine the nature of the contacts. These effects on the molecular level are able to trigger macroscopic morphological changes of the adsorbed material.
Using atomistic simulations in the area of force field and density functional applications, I will highlight the role of specifically water and ions as well as the local surface charge distribution on adsorption processes using selected examples of protein - protein and protein - bioceramics interfaces. Namely, I will talk about the comparative adsorption of lysozyme, chemotrypsin and fibronectine [Figure1] on three different oxides (SiO_2, TiO_2 and Al_2O_3) which span a wide range of PZCs [1-4].

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FIGURES

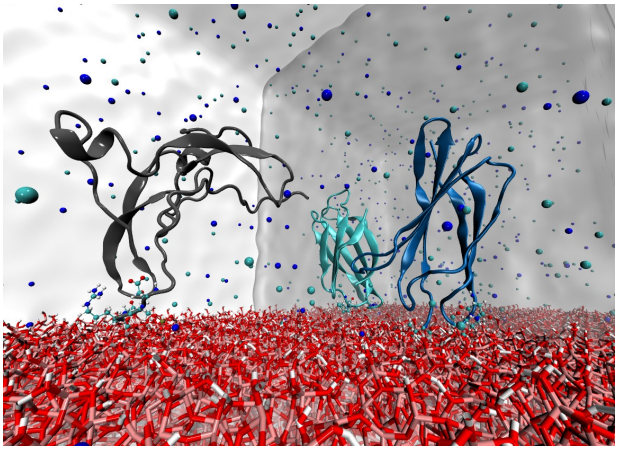

Figure 1: The C-terminal interchain domain of fibronectine (gray), as well as the modules 10FnIII (cyan) and 7FnIII (blue) in an aqueous ionic solution adsorbed on an amorphous alumina surface. The visible liquid wall in the background indicates the size of the simulation cells