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Solid-liquid multiphase simulation of protein-surface interaction and protein adsorption on polymer surfaces

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Understanding protein-surface interaction and protein adsorption properties of polymer surfaces are of crucial importance for the use of polymers in biomedical implants. Though polymer surfaces do not provide any receptors for cellular proteins, soluble proteins can bind to these polymer surfaces and in turn act as receptors for cellular proteins. In the process, depending on the surface properties of the polymer, the bound proteins can assume unrecognizable conformations allowing cellular proteins to identify them as foreign bodies and trigger attacks as a cellular response. These infighting posses a major challenge in biomedical engineering. An appropriate understanding of the adsorption free energy and the conformational changes of proteins upon their interaction with synthetic surfaces is critical in the development of biomaterials suitable for implants because those changes determine cellular responses to implanted materials and substrates. The classical molecular dynamic (MD) simulation is one of the direct methods which can, in principle, provide a detail analysis of the molecular behavior of the protein-surface interaction. However, there are challenges from the compatibility of the force-field parameters that needs to be overcome. MD force-field parameters developed for liquid phase proteins and solid phase surfaces serve well for the respective phases but the interphase interaction between a surface and a protein or water appear to be inappropriate and the scale of inadequacy vary significantly based on the hydrophobicity of the surface. To circumvent this situation, we developed a dualFF formalism in CHARMM, where dedicated parameter sets are being used for the solid phase surface and the liquid phase protein and water but to describe the interphase interaction between protein-surface and water-surface a third set of parameters are used which are tuned to respond to the polarization effect on the liquid phase protein and the water in the presence of the solid phase surface. Simulation results for peptide adsorption on self-assembled monolayer surfaces with hydrophobic and hydrophilic functionalized groups will be presented with untuned and tuned interphase force-filed parameters and compared with experimental data. Results demonstrate the suitability of the dualFF method to characterize protein-surface interaction and designing appropriate functionalized surface for biomedical implants.

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