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Surface Stress Calculations of Bio-molecular Adsorption on Gold-coated Micro-cantilever Biosensor Using Molecular Dynamics Simulation

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Micro-cantilever biosensors are one of the rapidly developing biosensors with numerous advantages like high sensitivity, wide applicability and low cost. It can detect various specific bio-recognitions by the surface stress induced bending of bio-molecular adsorption. To further advance the design of micro-cantilever biosensors, it is imperative to understand the mechanism of how bio-molecular adsorption influences the surface stress [1].

In this study, we used classical molecular dynamics simulation and two different bio-molecules to study the surface stress change of bio-recognitions. The EAM (embedded atom model) [2] potential, CHARMM force fields [3] and a hybrid interatomic potential were used to describe the gold surface, bio-molecular interactions and the interface between gold and biomolecules, respectively. We calculated the surface stress and entropy of single-stranded and double-stranded DNA adsorbed on the gold surface. We found that the surface change between single- and double-stranded DNA followed the same trend with the entropy change. It supports the previous assessment [4] that the entropy change is the key mechanism responsible for hybridization-induced surface stresses. The influence from ion concentration was also observed. To extend this approach to larger protein detection, the adsorption of prostate-specific antigen (PSA) was modeled. We found that the surface stress induced by bio-molecules is smaller than the thiol linker adsorbed on the surface by one to two orders.

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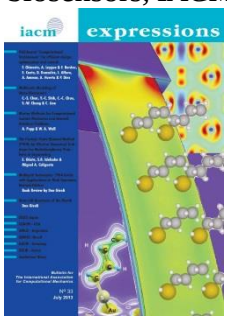

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