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Simulation of the Adsorption on Nano/Micro-Cantilever Sensors

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Recent advances in nano/micro fabrication techniques have led to the development of biosensors utilizing nano or micro-sized cantilevers. Through chemical coating of probe molecules that exhibit strong affinity to the target molecules, the cantilever would deflect when the target molecules bind with the probe molecules. Previous simulation studies on these systems often involved the use of a multi-scale approach in which molecular models are used for the probe and target molecules while the cantilever is modeled as a continuum solid beam using surface tension and strain energy. In this work, we use a molecular approach to describe the entire system. In particular, the solid beam is modeled as a collection of molecules connected by lattice springs. The intermolecular interactions between three types of molecules (i.e., probe, target and cantilever molecules) are modeled using Lennard-Jones potentials. Our results show that the cantilever deflection depend on the combination of the Lennard-Jones parameters as well as the number and positions of the probe and target molecules. Details of their effects will be presented in the paper.

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