139g Interaction between Model Proteins and Charge-Nanopatterned Surfaces: a Novel Multicanonical Simulation Approach

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The ability to recognize and handle individual biomolecules is of great technological importance and constitutes a major goal in Nanobiotechnology. Kan et al. (see Ref. 1) have developed a novel class of nanodevices with potential application in this field. They consist of arrays of metal nanoparticles embedded in a dielectric film. By controlling the amount of electric charges in each nanoparticle, non-uniform electrostatic fields with resolution in the nanometer scale can be created. In this work, we use molecular simulation to assess the ability of these devices to recognize and actuate specific biomolecules. For this, we study the thermodynamics of single protein molecules immersed in non-uniform electrostatic fields in the vicinity of a solid surface. A generalized Multicanonical Monte Carlo method is used to calculate variations in the system's free-energy as a function of the mean distance between the molecule and the surface. With this technique, trapping in free-energy local minima can be avoided, which is crucial in simulation of complex systems. At the same time, free-energy profiles and also average mechanical properties (such as mean molecular size) can be obtained for a range of temperatures in a single simulation. We found that the proximity of a neutral surface reduces the conformational entropy of a protein and promotes an increase in its folding temperature. This enhances the stability of the folded state and can decrease folding time, thus being a plausible explanation for the so-called “chaperone effect”. We also found that the non-uniform electrostatic fields created by a nanodevice can result in different binding free-energies for proteins with very similar masses and isoelectric points, but with distinct relative positions of charges within the molecular structure. This shows the potential of these devices to discriminate molecules which are very difficult to separate using conventional methods.

[1] Liu, Z.T., Lee, C., Narayanan, V., Pei, G., and Kan E.C., IEEE Transactions on Electron Devices 49, p. 1606, 2002.