Atomic Simulation of Lysozyme Adsorption on Hydrogen-Terminated Silicon Surface in Water

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Energy minimization and molecular dynamic (MD) simulations using explicit water model were carried out to gain insight into the adsorption behavior of lysozyme on hydrophobic hydrogen-terminated silicon (H-Si) surface in water medium. Bulk simulations were first preformed. The observed secondary structures are in substantial agreement with those from solution NMR data, indicating that the potential model is realistic. The protein deformation, internal structural rearrangements and global motions on the H-Si surface were then simulated. The results show that, in comparison with the configuration in bulk water, the lysozyme molecule undergoes deformation during adsorption on the hydrophobic surface, as is evidenced by the reduction in the volume (the radius of gyration, Rg), the increase in solvent accessible surface area (SASA), the change of the overall shape, and the alteration in secondary structures. The time evolution of the protein configuration shows significant internal structural motions while global motions are negligible over the simulation time scale. The main \(\alpha\)-helix domains experienced some loss while the \(\beta\)-sheet domains were almost unchanged. The hydrophobic character of the surface is believed to contribute to the loss of organized structures of the amino residues in close proximity to the surface.

Keywords:
Atomic Simulation, Adsorption, Lysozyme, Hydrogen-Terminated Silicon, Surface