Molecular Dynamics Simulation of BSA Adsorption on a Stepped Graphite Surface.

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Abstract

Carbon based structures such as pyrolitic carbon and graphene sheets are being used in the manufacturing of implant materials and bio-inspired sensors respectively due to the apparently good biocompatibility observed experimentally in these materials. In the case of defective surfaces composed of atomic steps embedded in solutions with low protein concentration, SPM studies show that the adsorption of protein occurs preferentially on the step edges, where a higher chemical reactivity is expected. It is therefore of a fundamental importance to understand how these highly reactive sites, influence the adsorption of protein in low concentration solutions.

To address this problem we have studied the adsorption of the serum-albumin, the most abundant plasma protein, onto a stepped graphite surface via molecular-dynamics atomistic simulations. The level of detail on our simulations such as the inclusion of explicit solvent and physiological ion concentrations allow us to address several open questions such as the influence on the protein adsorption properties (secondary structure, free energy, contact area, spreading and diffusion) upon the defect size (number of steps) and their nature.

References

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Figures

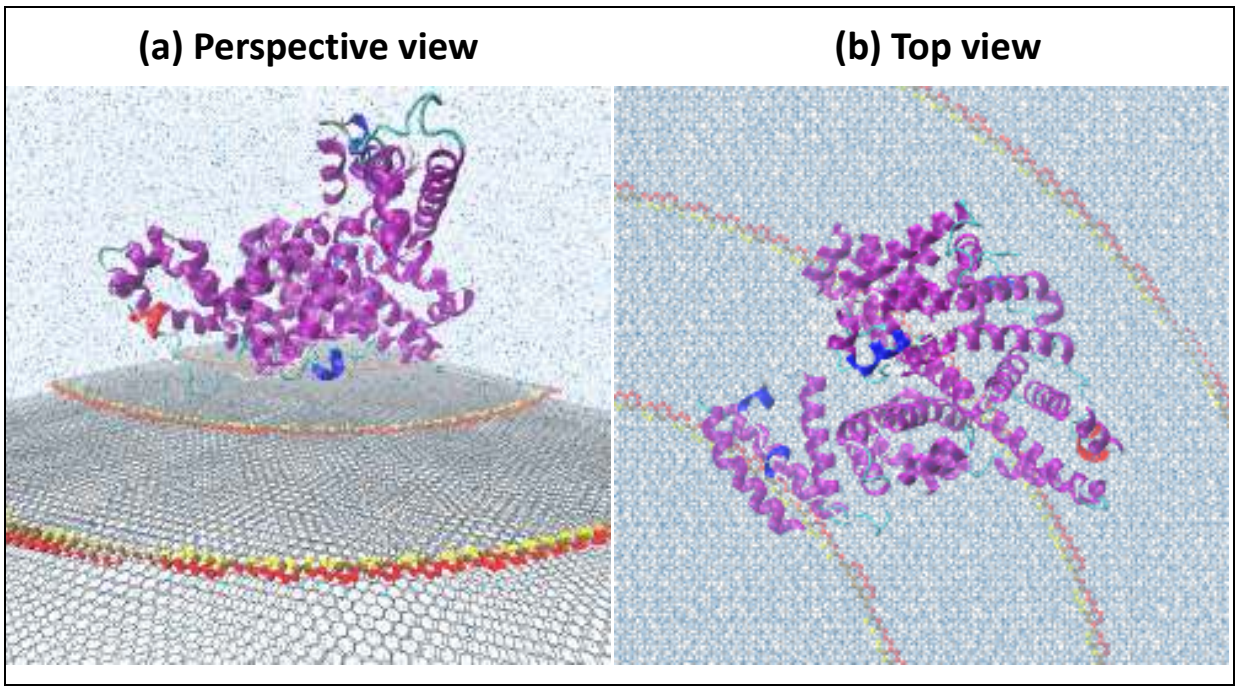

Figure 1. Bovine serum albumin (BSA) on top of a stepped graphite surface in explicit solvent. Atoms in step borders are depicted in color.