A molecular dynamics study of free and steered adsorption of BSA over graphene.

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Albumin, the most abundant plasma protein in mammals, is responsible of a manifold of vital functions. A better understanding of its adsorption over different surfaces would have a high impact on areas ranging from medicine to biochemical engineering [1,3]. Here, we study the Bovine Serum Albumin (BSA), which is the most widely used in experiments due to its low cost and its similarity to the human albumin. Recently it has been shown that graphene can be an optimal candidate to be used as an implant material [3]. Therefore the study of adsorption of BSA molecules on graphene will be of interest for addressing the use of graphene as biocompatible material.

Here we report a molecular dynamics (MD) study of the free and forced adsorption of BSA over graphene. The simulations were carried out using the AMBER force-fields [2] and both implicit as explicit solvent. This allows us to address several open questions: mechanisms behind the adsorption; role of the water molecules in the adsorption; the most favorable adsorption orientation. Furthermore, we demonstrate that BSA does not denature during adsorption if the solvent is explicitly included, at variance of recent findings [3].

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[2] J. Am. Chem. Soc. 117 (1995) 5179
[3] Langmuir 2011, 27, 12938.