

## Glucose adsorption on gold surface

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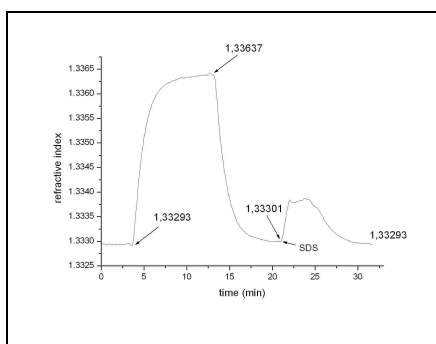
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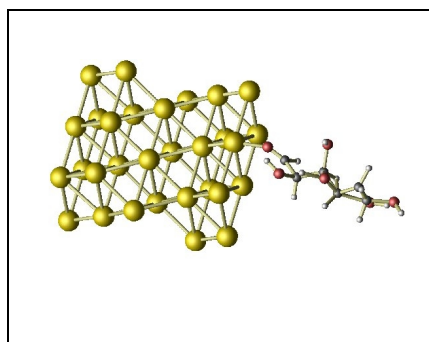
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**Abstract** – In this work, the adsorption of glucose on the gold (111) surface is investigated using surface Plasmon resonance and density functional theory calculations. The analysis of both theoretical and experimental data suggests that the adsorption of glucose on Au(111) takes place via the oxygen atom bonded to the free anomeric carbon of the glucose molecule.

Self-assembled monolayers are ordered molecular assemblies formed by the adsorption of an active surfactant on a solid surface. In particular, the immobilization of biomolecules has been used in biotechnological process, specially in the development of analytical sensors and hydrocarbon fuel cells[1-3]. Glucose is the most common carbohydrate and controlling its levels in are blood stream is not only related with the maintenance of life, but also with a number of serious diseases, like diabetes. The search for glucose biosensors has attracted a great deal of interest in the last decade. Different Au-based electrode biosensors have been proposed, but little is known about the interaction of glucose itself with the metal substrate. In this work, the interaction of glucose molecule with the gold (111) surface is studied by surface plasmon resonance (SPR) combined with density functional theory (DFT) calculations. Our experimental SPR data, represented in Figure 1, suggests that the adsorption of glucose on Au(111) takes place via the oxygen atom bonded to the free anomeric carbon of the glucose molecule in its cyclic chair or ring form. The different regimes represented in Figure 1 are as following: injection of the glucose solution in the chamber (increase in refraction index) dilution after water injection and injection of SDS 30~mM followed by water injection for the molecule desorption. SPR measurements of glucose and other polysaccharides indicate that their adsorption on gold only takes place in the presence of an anomeric carbon. Upon adsorption, the glucose rings open and the final adsorbed configuration resembles the linear form of glucose. This picture is supported by our density functional calculations, as for all considered adsorption sites (a-top, hollow and bridge) our simulations indicate the opening of the ring of the glucose molecule. Our theoretical calculations show that, after the cleavage of the O-H bond, the terminal oxygen makes a strong covalent bond to the surface indicating the formation of a chemisorbed monolayer mediated by the presence of an anomeric carbon, in agreement with the SPR measurements. In addition, other possible adsorption models and the adsorption coverage, i.e. the number of adsorbed molecules in the Au reconstructed surface, are investigated via SPR and DFT.



**Figure 1:** Index of refraction as a function of time for a 0.022g.mL<sup>-1</sup> glucose solution.



**Figure 2:** Schematic representation of glucose adsorption on Au(111) surface.



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