# THE ADSORPTION OF BIOMOLECULES ON GRAPHENE AND FLUORINATED GRAPHENES

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**Abstract**

Graphene and its derivatives found their usage in many fields of science due to the exceptional properties. In this work we focus on the theoretical description of the adsorption of three biochemical molecules (ascorbic acid, dopamine and nicotinamide adenine dinucleotide) on the surfaces of graphene and its fluorinated derivatives with various degree of fluorine coverage. Non-local correlation density functional that approximately accounts for dispersion interactions was used for prediction of adsorption geometries and adsorption energies of molecules on considered surfaces. Studied systems were compared and the most suitable surface for each molecule was chosen as recommendation for possible usage in construction of electrochemical sensors.

**Keywords:** Graphene, biosensing, density functional, fluorinated graphene, adsorption

**Author did not supply full text of the paper.**