## Accepted Manuscript

Design strategy of a graphene based bio-sensor for glucose

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PII: S0008-6223(18)30504-9

DOI: 10.1016/j.carbon.2018.05.044

Reference: CARBON 13171

To appear in: Carbon

Received Date: 16 January 2018

Accepted Date: 22 May 2018

Please cite this article as: Valentina Cantatore, Santosh Pandit, V.R.S.S. Mokkapati, Severin Schindler, Siegfried Eigler, Ivan Mijakovic, Itai Panas, Design strategy of a graphene based biosensor for glucose, *Carbon* (2018), doi: 10.1016/j.carbon.2018.05.044

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## ACCEPTED MANUSCRIPT

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## 17 Abstract

A novel graphene-based glucose sensor-design is formulated and explored in silico. An ad hoc 18 host molecule is tailored to bind to glucose by multiple hydrogen bonds. A pyridinic core is 19 chosen for this receptor in order to allow for "socket-plug" dative bonding to boron sites of 20 boron doped graphene. The modeling employs DFT (Density Functional Theory) together with 21 22 an effective aqueous environment to take into account the solvation effect. High selectivity is demonstrated for the suggested host molecule towards glucose as compared to other possible 23 competitors in blood such as fructose, biotin and ascorbic acid. A route to achieve improved 24 sensitivity, exploiting the hydrophilic/hydrophobic properties of the host+glucose system for 25 enhanced selective binding to the hydrophobic boron doped graphene support is discussed. 26

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