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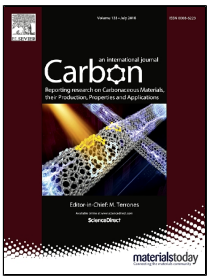

Design strategy of a graphene based bio-sensor for glucose

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Design strategy of a graphene based bio-sensor for glucose

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Abstract

A novel graphene-based glucose sensor-design is formulated and explored in silico. An *ad hoc* host molecule is tailored to bind to glucose by multiple hydrogen bonds. A pyridinic core is chosen for this receptor in order to allow for "socket-plug" dative bonding to boron sites of boron doped graphene. The modeling employs DFT (Density Functional Theory) together with 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 competitors in blood such as fructose, biotin and ascorbic acid. A route to achieve improved sensitivity, exploiting the hydrophilic/hydrophobic properties of the host+glucose system for enhanced selective binding to the hydrophobic boron doped graphene support is discussed.