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J Nanomed Nanotechnol 2018, Volume 9
DOI: 10.4172/2157-7439-C6-083

Electronic properties of various B-doped diamond (111)/dye molecule interfaces

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Diamond is a widely known material for its many excellent properties (e.g., high thermal conductivity, high break down voltage, transparency, chemical inertness and bio-compatibility). A B-doped diamond is an excellent p-type material for solar cell usage. Due to some specific properties (e.g., large chemical inertness, very high carrier mobility for both electron and holes and high transparency), it is considered as one of the strongest candidates for photovoltaic electric generation. However, in order to implement the usage of diamond in solar energy applications, properties like the electrochemical window, possibility for interfacial charge transfer and stability of functionalized surface, have been further studied and optimized. In the present investigation, the absorption of different dye molecules onto H-terminated diamond (111) surfaces, have been theoretically studied using Density Functional Theory calculations. The diamond surfaces were B-doped in order to make them p-type semi-conducting. The choice of dyes was based on the match between the electronic structures of these H-terminated B-doped diamond surfaces and the respective dye molecules. The dye molecules include $C_{26}H_{13}NO_3S_4$, $C_{35}H_{37}NO_2S_3$, $C_{34}H_{38}OS_2$, $C_{32}H_{36}OS_2$, and $C_{31}H_{35}S_3Br$. These dyes differ in the various functional groups, which have the role as electron acceptors. The main goal with the present study was thereby to investigate the photovoltaic efficiency of the various dyes when attached to B-doped and H-terminated diamond (111) surfaces. The calculated absorption spectra for in principle all of the different dyes were shown to be located in the most intense part of the sunlight spectrum. The usage of a combination of these different dyes would hence, be an optimal choice in order to improve the light harvesting in a photovoltaic process.

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