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

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 i) electrochemical window, ii) possibility for interfacial charge transfer, and iii) stability of functionalized surface, have be further studied and optimized. In the present investigation, the adsorption of different dye molecules onto H-terminated diamond (111) surfaces, have been theoretically studied using Density Functional Theory (DFT) calculations under periodic boundary conditions. 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 in the present study include $C_{26}H_{13}NO_3S_4$ (A), $C_{35}H_{37}NO_2S_3$ (B), $C_{34}H_{38}OS_2$ (C), $C_{32}H_{36}OS_2$ (D), and $C_{31}H_{35}S_3Br$ (E). 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 and compare the photo-voltaic efficiency of the various dyes when attached to B-doped and H terminated diamond (111) surfaces. Of a special interest was to study the i) absorption spectra of the dye, ii) degree of electron transfer over the diamond/dye interface, iii) electron transfer rate, iv) electron-hole recombination, and v) diamond/dye bond strength. 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. For the E dye, the spectrum was more positioned towards the UV light range. 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. Furthermore, the calculations identified the LUMO´s for the B, C, and D dyes to be positioned on the upper end of the molecules, which also will be the position of the electron acceptor when being excited by light. For the dyes A and E, there were though certain extensions of the LUMOs to the lower end of the molecules (i.e., towards the diamond surface), which will also increase the electron-hole recombination rates. Calculation of electron transfer was to ensure that the HOMO of these dyes was positioned at a lower energy compared to the upper edge of the valence band of the B-doped diamond surface. Moreover, all dyes were found to bind with strong C-C covalent bonds to the diamond (111) surface.

Biography

Karin Larsson is a Professor in Inorganic Chemistry at the Dept. of Chemistry-Ångström Laboratory, Uppsala University, Sweden, and a Guest Professor at the University of Science and Technology Liaoning, China. In addition, she is an Elected Member of IVA (Royal Swedish Academy of Engineering Sciences), division V (Mining and Materials; Vice-Chair). She is the Head of the Theoretical Materials Chemistry Group at the Div. of Inorganic Chemistry, Dept. of Chemistry-Ångström Laboratory. Her scientific focus is on interpretation, understanding and prediction of the following processes/properties for both solid/gas interfaces, as well as for solid/liquid interfaces; i) CVD growth (e.g. diamond, BN, and graphene), iii) interfacial processes for renewable energy applications (e.g. electrochemical processes), and iv) bio-functionalization of surfaces (e.g. bone regeneration).

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