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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. 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), it is considered as one of the strongest candidates for photovoltic 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 to 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. 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 included $C_{20}H_{13}NO_3S_4$ (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 photovoltaic efficiency of the various dyes when attached to B-doped and H-terminated diamond (111) surfaces. The calculated absortion spectra for in principle all of the different dyes were shown to be located in the most intense part of the sunlight spectrum.

Biography

Karin Larsson is working as a Professor of Inorganic Chemistry at the Department of Materials Chemistry, Uppsala University, Sweden. She is the Leader of the Theoretical Materials Chemistry Group at the Department of Materials Chemistry. 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 (incl. doping and its effect on surface properties), iii) interfacial processes for renewable energy applications (e.g. electrochemical processes), and iv) interfacial processes for e.g., bone regeneration (incl. biofunctionalisation of surfaces).

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