Computational studies on the effect of introducing a π-Bridge on the efficiency of a D-D-π-A system using DFT

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Abstract: The Dye-sensitized solar cell (DSSC) technology has developed as one of the most promising alternatives for renewable energy owing to the low cost, ease of manufacturing, and good conversion efficiency [1]. Till now, a variety of dye sensitizers have been explored, including the metal based as well as pure organic based solar cell devices [2, 3]. The metal free organic systems are better options owing to their low cost, easy availability and flexibility. We report DFT studies on some perylene based dyes for their electron transfer properties in solar cell applications. The study involves modeling of donor - donor - π - acceptor type sensitizers, with perylene and brazilein as donors and thiophene as the π-bridge. The effect of introducing a π-bridge as well as varying the π-bridges in this D-D-π-A framework was evaluated in terms of opto-electronic and photovoltaic parameters was carried out. All quantum computations were carried out using DFT using 6-311G (d, p) / LanL2DZ (for I and Ti atoms) as the basis sets and B3LYP as the functional, both in the gas phase as well as solvent phase, with Gaussian 03 set of codes. We found that the sensitizers exhibited good optical as well as photovoltaic response with PB2, PB7, PB8 and PB9 having benzene, pyrimidine, pyrazine and aniline as π-bridges, exhibiting better electron injection efficiencies (Fig.1) and hence expected to be better sensitizers. The overall opto-electronic and transport parameters of the TiO_2 - dye adsorbed systems after anchoring the dyes on the model TiO_2 cluster was also studied

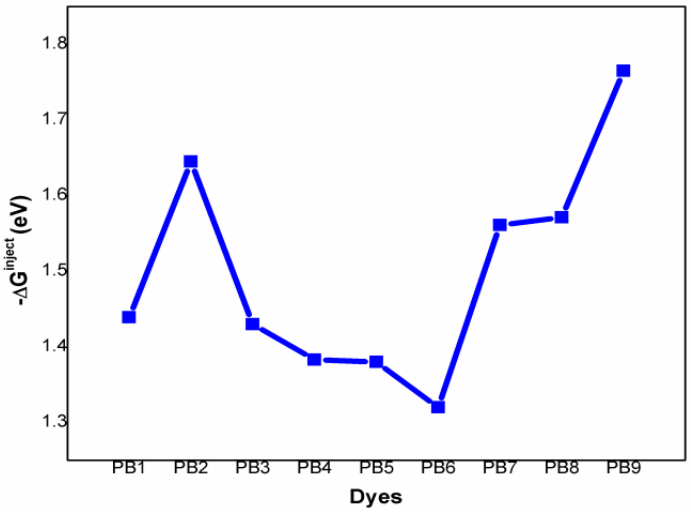

Figure 1: Calculated electron injection efficiencies of various dye sensitizers.

References:

1. O'Regan, B.; Gratzel, M. Nature, 1991, 35, 737−740.
2. Chung, I.;. Lee, B.; He, J.; Chang, R. P. H.; Kanatzidis. M. G.; Nature, 2012, 485, 486 – 489.