Benzimidazole based Organic Dyes Containing Nitro Group as an Acceptor/Anchoring Group for Dye Sensitized Solar Cells Applications

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Abstract— *In the past two decade, tremendous efforts had been devoted to improve the performances of DSSCs and to increase their commercial attractiveness by using several different classes of materials. Among them, sensitizers play a major role. For this reason many efforts have recently focused on the development of new efficient organic dye molecules with good photoelectrical properties through simple synthetic routes. Most of the organic dyes have a donor-π-acceptor (D-π-A) architecture. For this, benzimidazole derivatives were chosen as π-linker and as well as acceptor since which are well known for their low cost, simple synthesis, electron transporting ability, thermal and chemical stability. In this concern, 5-nitro benzimidazole based new four organic dyes were synthesized through the Vilsmeier-Haack formylation, condensation of corresponding aldehyde with substituted o-phenyline diamine lead to benzimidazole formation and Knoevenagel condensation reactions. The electronic and structural properties of the dyes were investigated by UV-vis and fluorescence spectroscopy. To establish an optimized structure and HOMO-LUMO of dyes, DFT calculations were performed at a B3LYP/6-31G(d) level. Theoretically calculated*

LUMO values of all dyes were in the range of -2.33 to -2.99 eV, which is more negative than the conduction band of TiO2. This suggests that the effective electron transfer from the excited dye to TiO2 is energetically feasible. The HOMO values of dyes were in the range of -5.46 to -5.12 eV. This value is more positive than the redox couple (I-/I3-) and so this favours the dye regeneration by the electrolyte. From this study all synthesized molecules were act as a good photosensitizer for DSSC applications.