An experimental and DFT study on novel dyes incorporated with natural dyes on titanium dioxide (TiO$_2$) towards solar cell application

Muhammad Kashif[1] · Zainab Ngaini[2] · Angelina Viviana Harry[3] · Rohit L. Vekariya[4,5] · Awais Ahmad[6] · Zhiqiang Zuo[1] · Siti Kudnie Sahari[7] · Shahid Hussain[8] · Zuhaib Ashfaq Khan[9] · Abdullah Alarifi[10]

Abstract

Titanium dioxide (TiO$_2$) thin films were deposited on fluorine tin oxide (FTO) coated glass substrate using spin-coating techniques and as-deposited films were sensitized with various dyes. A series of azo derivatives (2, 5a-b) having different structures were successfully prepared through the process of the azo coupling reaction. KAZO 6 was successfully synthesized by esterification of kojic acid obtained from sago waste with azo 5a. These azo dye were examined using density functional theory (DFT) and time-dependent density functional theory (TD-DFT) to obtain the vertical excitation, electron distribution, energy levels, band gap, and light-harvesting efficiency in the ground and excited state. The obtained values exhibited a good correlation with the experimental values. Efficiency enhancement was reported by the incorporation of KAZO 6 with curcumin extracted from turmeric. Spectroscopy and optical properties of synthesized dyes were characterized using CHNS elemental analysis, FTIR, ^{1}H NMR, ^{13}C NMR, and UV–Vis spectroscopies. KAZO 6 displayed an efficiency of 1.59% compared to azo derivatives 0.13–1.12%. The efficiency of KAZO 6 enhanced from 1.59 to 1.74% with the incorporation of turmeric dye.

Graphic abstract
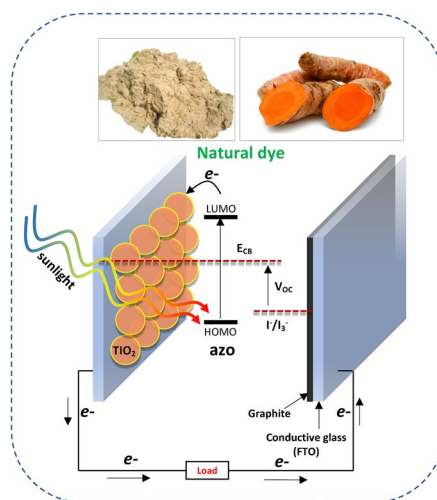
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