



An experimental and DFT study on novel dyes incorporated with natural dyes on titanium dioxide (TiO₂) towards solar cell application

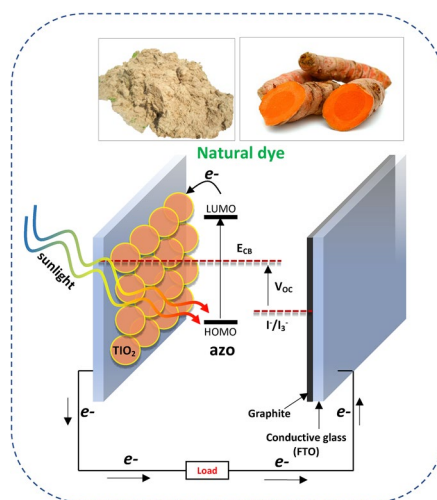
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Abstract

Titanium dioxide (TiO₂) 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, ¹H NMR, ¹³C 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



Keywords Azo derivatives · KAZO 6 · Turmeric · Spectroscopic · Optical · Electrical · DSSC

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