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Effect of methoxy functionalized group on the photocatalytic properties of diphenylaniline organic Chromophores

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Diphenylaniline dyes are important sets of organic dyes that has stirred many research interest as photosensitizers in TiO2 semiconductor based dye sensitized solar cells (DSSCs). The advantages of organic dyes over metal based complexes are higher extinction coefficient, low cost, good environmental compatibility and electrochemical properties. The diphenylaniline organic dyes with basic configuration of donor-π-acceptor are relatively cheap, easy to synthesize and possess chemical structures that can easily be altered to optimize their photocatalytic properties. The enormous interest in dipheylaniline dyes as photosensitizers is due to their fascinating spectral properties which include visible light to near infra-red light absorption. In this work, density functional theory approach via GPAW, Avogadro and ASE were employed to study the effect of the methoxy functionalized group on the spectral properties of diphenylaniline dyes to improve their photocatalytic properties to harness more near infrared photons. Our results shows that the two dyes with pure phenyl groups D5 and D7 shows maximum absorption peaks at 750 nm and 850 nm, while D9 and D11 with methoxy group shows maximum absorption peak at 800 nm and 900 nm respectively. The highest absorption wavelength is notable for D9 and D11 containing methoxy groups. Also D9 and D11 dyes with the methoxy group shows lower energy gap of 0.98 and 0.85 respectively than the corresponding D5 and D7 dyes with energy gap of 1.32 and 1.08. The analysis of their electron injection kinetics ΔGinject into the band gap of TiO2 shows that D9 and D11 with the methoxy group has higher electron injection kinetics of -2.070 and -2.030 than the corresponding pure phenyl dyes with ΔGinject values of -2.820 and -2.130 respectively. Our findings suggest that the photocatalytic properties of organic chromophores with donor-π-acceptor configuration can be enhanced by the addition of functionalized groups.

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No

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