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Effect of Methoxy and Polyene Additional Functionalized Group on the Photocatalytic Properties of Polyene-Diphenylaniline Organic Chromophores for Solar Energy Applications

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Abstract : The global potential of other renewable energy sources such as wind, hydroelectric, bio-mass, and geothermal is estimated to be approximately 13 %, with hydroelectricity constituting a larger percentage. Sunlight provides by far the largest of all carbon-neutral energy sources. More energy from the sunlight strikes the Earth in one hour (4.3 × 1020 J) than all the energy consumed on the planet in a year (4.1 × 1020 J), hence, solar energy remains the most abundant clean, renewable energy resources for mankind. Photovoltaic (PV) devices such as silicon solar cells, dye sensitized solar cells are utilized for harnessing solar energy. Polyene-diphenylaniline organic molecules are important sets of molecules that has stirred many research interest as photosensitizers in TiO_2 semiconductor-based dye sensitized solar cells (DSSCs). The advantages of organic dye molecule over metal-based complexes are higher extinction coefficient, moderate cost, good environmental compatibility, and electrochemical properties. The polyene-diphenylaniline organic dyes with basic configuration of donor-π-acceptor are affordable, easy to synthesize and possess chemical structures that can easily be modified to optimize their photocatalytic and spectral properties. The enormous interest in polyene-diphenylaniline 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 software, Avogadro and ASE were employed to study the effect of methoxy functionalized group on the spectral properties of polyene-diphenylaniline dyes and their photons absorbing characteristics in the visible region to near infrared region of the solar spectrum. Our results showed that the two-phenyl based complexes D5 and D7 exhibits 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 additional polyene and methoxy groups. Also, D9 and D11 chromophores with the methoxy group shows lower energy gap of 0.98 and 0.85 respectively than the corresponding D5 and D7 dyes complexes with energy gap of 1.32 and 1.08. The analysis of their electron injection kinetics ΔGinject into the band gap of TiO_2 shows that D9 and D11 with the methoxy group has higher electron injection kinetics of -2.070 and -2.030 than the corresponding polyene-diphenylaniline complexes without the addition of polyene group with ΔGinject values of -2.820 and -2.130 respectively. Our findings suggest that the addition of functionalized group as an extension of the organic complexes results in higher light harvesting efficiencies and bathochromic shift of the absorption spectra to higher wavelength which suggest higher current densities and open circuit voltage in DSSCs. The study suggests that the photocatalytic properties of organic chromophores/complexes with donor-π-acceptor configuration can be enhanced by the addition of functionalized groups.

Keywords : renewable energy resource, solar energy, dye sensitized solar cells, polyene-diphenylaniline organic chromophores
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