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A Comprehensive Study of the Optoelectronic Properties of Donor-Acceptor Based Derivatives of 1,3,4-oxadiazole

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Abstract

A variety of 1,3,4-oxadiazole derivatives based on electron- donor pyrrole and -acceptor nitro groups are modelled. Various isomers of pyrrole-oxadiazole-nitro unit and its dimer linked to substituted and unsubstituted phenyl group are studied using the dispersion corrected density functional theoretical method. The electron density distribution in frontier orbitals of the phenyl-spacer compounds bearing amino and phenylamino groups indicates the possibility of intramolecular charge transfer. The isomers of phenyl-spacer compounds absorb in visible region of electromagnetic spectrum. The compounds show high values of light harvesting efficiency, despite the weak anchoring nature of nitro groups.

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