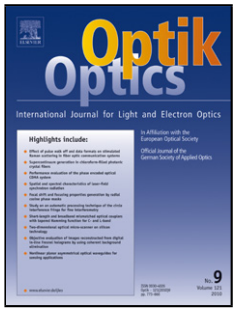

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Tuning of optoelectronic and charge transport properties in star shaped anthracenothiophene-pyrimidine derivatives as multifunctional materials

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Abstract

With the aim to tune the optoelectronic, charge transport and nonlinear optical properties, four novel star shaped compounds were designed from the initial structure 4,6-di(anthracenothiophen-2-yl)pyrimidine (DATP). The (2,5-di-(thiophen-2-yl)-4,6-di-(anthracenothiophen-2-yl)pyrimidine) (**1**), (2,5-di(benzo-thiophen-2-yl)-4,6-di-(anthracenothiophen-2-yl)pyrimidine) (**2**), 2,5-di(naphthothiophen-2-yl)-4,6-di-(anthracene-thiophen-2-yl)-pyrimidine (**3**), and 2,4,5,6-tetrakis(anthracene-thiophen-2-yl)pyrimidine (**4**) were deliberated by substituting the thiophene, benzothiophene, naphthothiophene and anthracenothiophene moieties at positions 2 and 5 of the pyrimidine unit in DATP, respectively. The ground and excited state geometries were optimized by adopting the density functional theory (DFT) and time-dependent DFT at B3LYP/6-31G** and TD-B3LYP/6-31G** level of theories, respectively. We shed light on the energies of the frontier molecular orbitals (FMOs), energy gaps (E_{gaps}), absorption, fluorescence, total/partial density of

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