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Luminol Modified Polycarbazole and Poly(o-anisidine): Theoretical Insights Compared with Experimental Data

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Abstract

With the aim to explore the effect of luminol as a multifunctional dopant for conjugated polymers, the present study reports the ultrasound-assisted doping of polycarbazole (PCz) and poly(o-anisidine) (PANis) with luminol in basic, acidic and neutral media. The synthesized homopolymers and luminol doped polymers were characterized using FT-IR, UV-visible and XRD studies while the photo-physical properties were investigated via fluorescence spectroscopy. Density functional theory (DFT) calculations were performed to get insights into the structural, optical, and electronic properties of homopolymers of polycarbazole (PCz) and poly(o-anisidine) (PANis). Vibrational bands B3LYP/6-311G (d,p) level, UV-vis spectral bands and electronic properties such as ionization potentials (IP), electron affinities (EA)

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