

Structural and electronic properties of FeO-decorated polythiophene-poly 3-methylpyrrole composite copolymer: DFT study

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The current study investigates the structure and electronic properties of the FeO-decorated polythiophene-poly 3-methylpyrrole composite copolymer using a density functional theory-based *ab initio* approach. The synthesized composite copolymer has a high stability with a binding energy of -5.2 eV compared to polythiophene-poly 3-methylpyrrole copolymer. The synthesized copolymer exhibits a 58.5% reduction in bandgap due to the formation of composite with FeO, and increased conductivity. The structural and electronic properties of FeO decorated polythiophene-poly 3-methylpyrrole composite copolymer are analysed *via* electron density, density of states, HOMO-LUMO gap, and Mulliken population. The enhanced conductivity and stability of the FeO-decorated composite copolymer make it a promising candidate for various applications, including polymeric sensors, energy storage, photovoltaic and electronics devices.

Keywords: Composites, Electronic properties, Sensor applications, Stability, Copolymerization