

Improvement of performance of electronic devices based on polythiophane by using band gap engineering in the presence of graphene

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Abstract

Density functional theory (DFT) and many body perturbation theory at the G_0W_0 level were used to investigate the change of the electron properties of Polythiophene (PT) polymer in the vicinity of graphene. The result of the analysis of the change in the density of the load compared to the pre-mutual interaction indicates a strong electric bipolarity and an absorption of the physical type at the surface. The change in the calculated electrical potential indicates the change in the work function to the value -0.19 eV of its initial value 4.53 eV . The results from the DFT do not show a change in the polymeric energy gap, while graphene energy gap changes from the isolated chain obtained from the results of the many body perturbation theories at the G_0W_0 level.

Keywords: Work function, Band structure, Physisorption, Electron charge density, Electric bipolarity, Many body perturbation theory

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