



A Combined Experimental and Theoretical Study of Optoelectronic and Structural Properties of a New Copolymer Based on Polyvinylcarbazole (PVK) and Poly (3-hexylthiophene) (PHT)

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Abstract

In this paper we report on a combination of experimental and theoretical study of a new copolymer based on carbazole and methylthiophene (Cbz-Mth), in their neutral and oxidized states. We discuss the influence of chain length on conformational and optoelectronic properties with the DFT method. Conformational analysis shows that there are no big changes in the structural parameters of neutral oligomers. In the doped form, the oligomer structures become nearly planar and show a quinoidal character. The results obtained for (Cbz-Mth)₃ from the neutral state, are close to experimental values. Key words: (Cbz-Mth) oligomers; DFT; Conformational analysis; Optoelectronic properties; Polaronic and bipolaronic forms.

Introduction

Enormous efforts have been made toward the development of conjugated polymers as light-emitting diodes [1-3] and field-effect transistors (FET) [4]. In the categories of conjugated polymers, polythiophene and derivatives have been studied extensively due to their good stability both in neutral and

doped states and their wide electronic and optical tuning [5-7]. The electric properties of polythiophenes are strongly governed by the intramolecular delocalization of π -electrons along the conjugation chain. This delocalization depends on the extent of the overlapping between the pz orbitals of the carbon atoms in positions α and α' of adjacent

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