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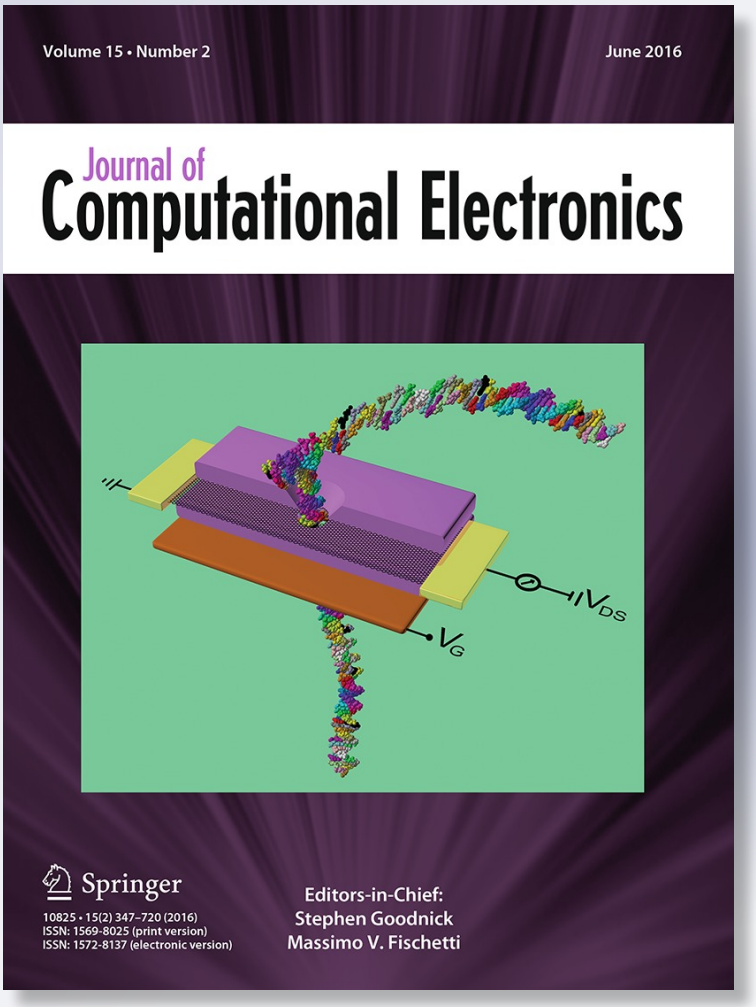

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The Monte Carlo simulation of the hole transport in thin films of PFO:MEH-PPV

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Abstract Hole transport is numerically studied by means of the Monte Carlo method in a single blended layer of poly(9,9′-dihexyl fluorenyl-2,7-diyl) (PFO) and poly(2-methoxy-5-(2-ethylhexyloxy)-l,4-phenylenevinylene) (ME H-PPV), which is sandwiched between two electrodes. A bimodal Gaussian density of states is used for randomly distributed localized states in the blended organic layer and an exponential distribution function for trap density of states. In this study, a new approximation has been used for the Fermi level instead of the Boltzmann approximation due to the high charge carrier density. The current density and the mobility have been calculated for different concentrations of MEH-PPV versus voltage and 1000/T at temperatures 150–290 K. The results of calculations show that the current density and the mobility are maximized at the blending ratio of 2 wt%, and there is a linear relationship between the current density and 1000/T at different voltages. The comparison of the numerical results with the experimental data shows a very good consistency between them, particularly at low and medium voltages of the working range of organic semiconductor devices.

Keywords Charge transport · Monte Carlo · PFO:MEH-PPV blend · Bimodal method · Thin film

1 Introduction

Organic semiconductors including conjugated polymers and small molecules are the promising materials which have attracted attentions of many researchers. These materials are increasingly used in different devices such as organic light emitting diodes (OLED), thin film transistors (TFTs), solar cells, etc [1–9]. Poly (9,9′-dihexyl fluorenyl-2,7-diyl) (PFO) and poly (2-methoxy-5-(2-ethylhexyloxy)-l,4-phenylenevinylene) (MEH-PPV) are two important substances among these materials. Polyfluorene (PFO)-based organic semiconductors and their derivatives have a high carrier mobility, and their emission is in and around the blue region, therefore, these materials have a good perspective being applied in polymer LEDs (PLEDs) and photovoltaic devices [1–3,10]. The derivatives of poly(*p*-phenylene vinylene) (PPV) including MEH-PPV, in turn, are the materials that usually have high photoluminescence yields and high values of the hole mobility [11], and consequently, they are regarded as suitable semiconductors for LEDs [12]. The optical and electrical properties of these materials have been widely studied experimentally and numerically on their own [13–17].

One can modify and regulate the optical and electrical properties of a material by blending it with other materials in the forms of host–guest systems. This has been extensively investigated by researches over the past years [18–22]. The PFO:MEH-PPV blend has received less attention especially in a numerical manner, although PFO and MEH-PPV have been extensively studied when they are blended with other materials.

Ananthakrishnan et al. [23] examined the tuning emission color in a ternary blend of PFO and MEH-PPV in an inert matrix polymer PMMA host. They showed that electroluminescence efficiency increases as a small concentration of MEH-PPV is blended with PFO, and the emission color of the structure changes as the voltage changes due to the micro- and nano-phase-separated domains in the blend [23]. Recently, Bajpai et al. [24] have experimentally studied the current

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