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Title: Variations in the optical properties of poly(3-hexylthiophene)/C_{60} blends and poly(3-hexylthiophene)/sol-gel composites

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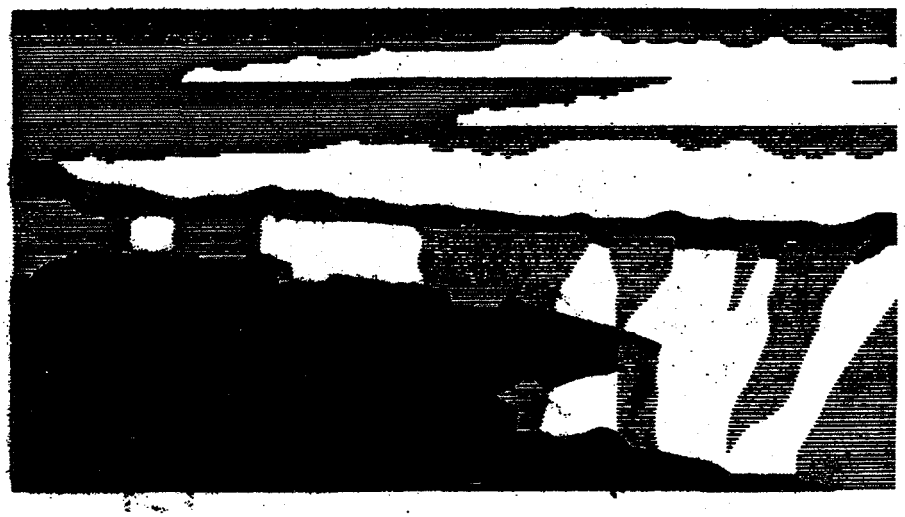

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Variations in the optical properties of poly(3-hexylthiophene)/C_{60} blends and poly(3-hexylthiophene)/sol-gel composites

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Abstract

We report the synthesis and characterization of thin films of poly(3-hexylthiophene) (P3HT)/C_{60} blends. UV-Vis spectra of the P3HT/C_{60} blends with various amounts of C_{60} show significant blue shift, which indicates the complex formation between P3HT and C_{60}. A new type of luminescent glass was also prepared by sol-gel technique. This method allows incorporation of P3HT (photoemissive polymer) into the sol-gel matrix and results in glasses that feature stimulating photoluminescent properties. By slightly varying the synthetic conditions of fabricating these P3HT/sol-gel glasses, we can control their emission colors from blue to red, covering the whole visible spectrum.

Keywords: Poly(3-hexylthiophene), Fullerene, Photoinduced absorption, Photoluminescence, Sol-gel

1. Introduction

Long alkyl chain on the 3-position of the thiophene ring allows poly(3-hexylthiophene) to be soluble in most of common organic solvents, such as xylene, tetrahydrofuran, *etc*. Solution processing allows fabrication of P3HT into thin films and devices for studying their electronic and optical properties of P3HT [1] and in its composites with fullerene [2]. So far, few studies on the topic of effect of polymer conformation [3, 4] show encouraging results for fine-tuning the electronic and optical properties of conducting polymers. In this paper, we report the synthesis and characterization of thin films of P3HT/C_{60} blends. We also report the synthesis of P3HT/sol-gel glasses, which emit visible light from blue to red, covering the whole visible spectrum. This is the first time (to our knowledge) when a single photoemissive polymer is shown to radiate different colors of light in the visible region, which is achieved by simply varying the reaction parameters of the sol-gel synthesis. This novel approach shows promise for applications in light emitting diodes.

2. Experimental

Poly(3-hexylthiophene) was prepared and purified according to the literature procedure [5]. Both P3HT and C_{60} were dissolved in xylene to give 2 mg/ml solutions. Thin films of P3HT/C_{60} blends were prepared by mixing poly(3-hexylthiophene) and C_{60} solutions with appropriate molar ratio and subsequently spin-casting and/or drop-casting on a quartz plate. P3HT/sol-gel composites were prepared by a method similar to [6], using dichlorobenzene as cosolvent.

Absorption spectra were measured by a Perkin-Elmer Lambda 19 UV-Vis-NIR spectrometer. Photoluminescence (PL) spectra were obtained by exciting with 400 nm light and collecting the fluorescence using a CCD spectrometer.

3. Results and discussion

3.1. Poly(3-hexylthiophene) and C_{60} blends

Figure 1 shows the UV-Vis spectra of the P3HT/C_{60} blends with different C_{60} concentrations in the blends. Blue shift of the λ_{max} was observed with the increasing amount of C_{60} incorporated with the P3HT, up to 20% *w/w*.

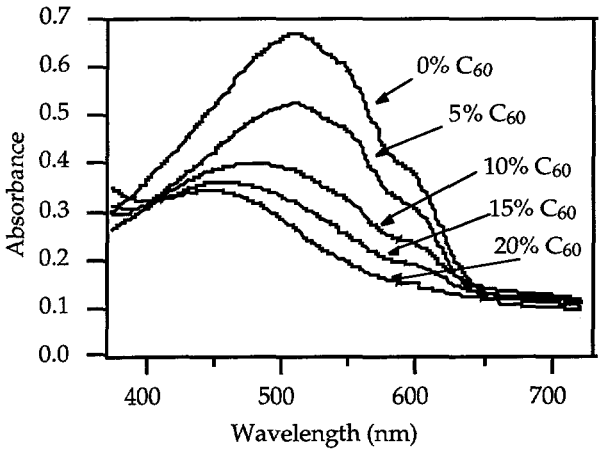

Figure 1. UV-Vis spectra of the P3HT/C_{60} blends with different C_{60} concentrations in the blends.

We believe that this blue shift is due to the formation of P3HT/C_{60} complex in which C_{60} molecules interact with the polymer chains thus altering the P3HT conformation, shortening the effective conjugation length and/or reducing delocalization of electrons on the P3HT backbone structure. A similar blue shift of the PL spectra with increasing C_{60} concentration in P3HT has been reported [7]. This agrees well with our results in Fig. 1. Lack of the absorption in the near-infrared region suggests that there is no noticeable ground state charge transfer between P3HT chains and C_{60} molecules.

3.2 Poly(3-hexylthiophene) and sol-gel composites

The P3HT sol-gel composites were successfully prepared in a wide range of concentrations. Figure 2 shows

the UV-Vis spectra of the P3HT solution, thin film and sol-gel composite that have λ_{max} at 454 nm, 502 nm and 405 nm, respectively. The distinctive blue shift in UV-Vis spectrum of P3HT/sol-gel composite (405 nm) as compared to that of the solution (454 nm) and thin film (502 nm) indicates that polymer conformation was altered by the strong dielectric difference between the P3HT and inorganic sol-gel polymers. Absence of the shoulder peak at 454 nm and 502 nm suggests that homogeneous solid solution was formed without aggregation of the polymer in the sol-gel matrix.

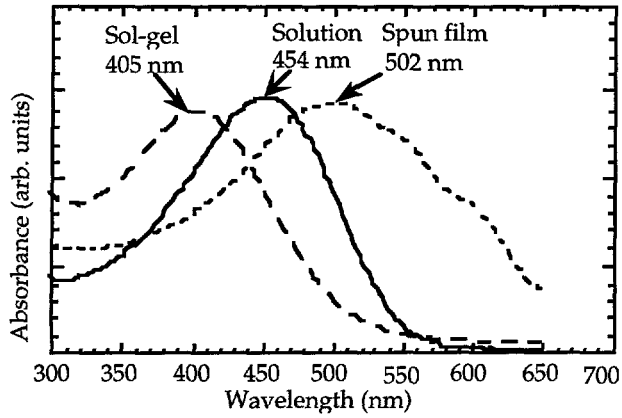

Figure 2. UV-Vis spectra of P3HT in dichlorobenzene solution, spun film from dichlorobenzene, and in sol-gel composite.

By varying the reaction parameters, we were able to fine-tune the absorption spectra of the P3HT in the sol-gel matrix which results in different photoluminescent properties, as shown on Figure 3. Two composites with absorption λ_{max} at 412 and 426 nm emit yellowish light with λ_{max} at 565 nm and orange light with λ_{max} at 585 nm, respectively. We have been able to expand the luminescence spectra of the P3HT/sol-gel glasses, so that they cover all visible spectrum from blue to red (data not shown here). We believe that P3HT may have very different conformations in the sol-gel glass matrix which leads to dramatic variance in their absorption spectra, λ_{max} ranges from 365 nm to 426 nm.

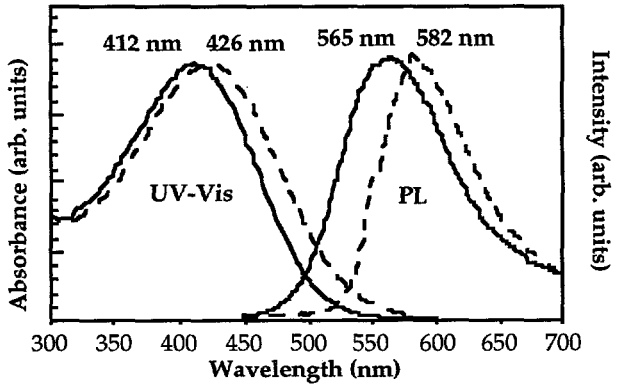

Figure 3. Selected examples of UV-Vis and photoluminesence spectra of poly(3-hexylthiophene)/sol-gel glasses.

Conclusions

We have found that formation of the complex between P3HT and C_{60} lead to the significant conformational changes in the polymer, causing considerable blue shift in the UV-Vis spectra of the P3HT/C_{60} blends.

Using our sol-gel processing technique we have prepared a new type of luminescent glass, P3HT/sol-gel composites. These composites emit colors from blue to red which encompass the whole visible spectrum.

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