# Charge carrier transport in blend of P3HT and ZnO nanoparticles at low temperature studied by μSR

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# Charge carrier transport in blend of P3HT and ZnO nanoparticles at low temperature studied by μSR

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**Abstract.** Recently, hybrid solar cell, which is a combination of organic and inorganic material, has been developed to produce better performance especially in power conversion efficiency of solar cell. Organic material based on conjugated polymer such as Poly(3-hexylthiophene) (P3HT) attracted much attention because P3HT shows the highest hole mobility among the series of Poly(3-alkylthiophene). On the other hand, it is well known that ZnO nanoparticles are an inorganic material with high electron mobility that can be acted as electron acceptor to dissociate excitons formed in organic material. The existence of ZnO nanoparticles in active layer of solar cell will lead to dissociation of excitons in P3HT via rapid electron transfer to ZnO. To understand the mechanism of charge carrier transport in blend of P3HT and ZnO nanoparticles, we have been conducted an experiment using muon spin relaxation (μSR) at low temperature of 10 K with variation of longitudinal field from 2 to 395 mT. We also investigated the effect of light irradiation to the charge carrier transport in blend of P3HT and ZnO nanoparticles. Without light irradiation, it is clearly observed that depolarization rate (λ) was proportional to linier field of $H^{-0.5}$, indicating one-dimensional intra-chain transport of charge carrier. With light irradiation, it is found that asymmetry data changed slightly indicating the trace of any changing of charge carrier transport to increase in the amount of exciton in samples causing by light irradiation.

## 1. Introduction

Organic solar cells have attracted much attention because of their potential in the low-cost production of solar panels, featuring a flexible, lightweight, and ultrathin device. The power conversion efficiency (PCE) of organic solar cells is now reaching up to 10% [1] and it could be improved by modifying the active material of solar cells. Poly-(3-hexylthiophene) (P3HT) is a polymer, which is widely used as active material in photovoltaic devices [2]. P3HT has considerable attracted research interest because P3HT shows the highest hole mobility compared to other conjugated polymers [3].

Recently, many researchers give attention to hybrid solar cells to improve performance of solar cells whilst still maintain low cost processability [4]. Hybrid solar cells consist of organic materials, normally conjugated polymer that absorb light as the donor and inorganic materials as the acceptor

and electron transporter in the structure. ZnO as inorganic material has some advantages such as having high electron mobility, becoming one of candidates to be combined with organic material of P3HT in active layer of hybrid solar cell. The advantage of P3HT mixed with ZnO nanoparticles give a promising material for better performance of hybrid solar cells [5]. ZnO prepared as nanoparticles resolve the problem of small diffusion range of P3HT [6]. The existence of ZnO in active layer will support charge transfer from P3HT to electrode of solar cell. The phenomena could be realized due to the conduction band of ZnO is lower than that of low unoccupied molecular orbital (LUMO) of P3HT as shown in figure 1.

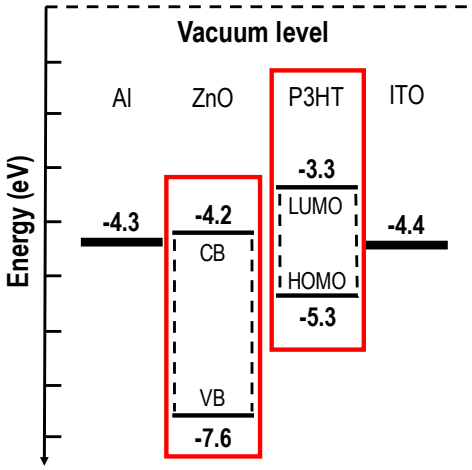


**Figure 1.** Energy level of P3HT and ZnO.

We have studied the microscopic intrinsic charge carrier dynamics in active material of P3HT:ZnO blend of hybrid solar cells along and perpendicular to the chain by using the longitudinal field (LF) μSR method. Figure 2 shows the longitudinal field dependence of $\lambda_1$ in P3HT:ZnO [7]. We found that the charge carrier mobility changes from intra-chain diffusion that charge diffused along the polymer chain to inter-chain diffusion that charge diffused in between the polymer chain. One-dimensional intra-chain diffusion is observed in the samples at temperatures below 10 K, while three-dimensional inter-chain is observed at temperatures above 25 K. Compared with μSR data of P3HT that shows dimensional crossover at 25 K [8], it is apparent that the dimensional crossover from one-dimensional to three-dimensional in P3HT:ZnO is observed at lower temperature. ZnO nanoparticles facilitate the electron transfer from P3HT in blend of P3HT:ZnO more easily than in P3HT only.

In solar cells application, light was irradiated to initiate the charge carrier from P3HT as donor to ZnO nanoparticles as electron acceptor. In this paper, we performed light irradiation into sample of P3HT:ZnO to investigate the intra and inter-chain charge carrier dynamics by using longitudinal-field (LF) μSR. The results of charge carrier dynamics in active layer of P3HT:ZnO solar cell could be directly implied in fabrication of high performance of power conversion energy device.

## 2. Experimental methods

Conjugated polymer P3HT was obtained from Sigma-Aldrich without further purification. Sol-gel method was used to synthesize ZnO nanoparticles [9]. Hybrid organic-inorganic sample consisted of P3HT and ZnO nanoparticles were mixed by dissolving in chloroform and 3% methanol to produce a homogeneous solution. The solution was evaporated at 150°C to produce bulk of hybrid polymer P3HT:ZnO nanoparticles. For μSR measurement, P3HT:ZnO nanoparticles bulk sample was mounted on a silver plate in cryostat. The LF-μSR measurements were performed in magnetic field ranging from 0 to 395 mT at low temperature of 10 K. μSR measurements was carried out at the RIKEN-RAL Muon Facility, Rutherford-Appleton Laboratory, UK using a pulsed positive surface muon beam [10, 11]. White light source was irradiated to P3HT:ZnO nanoparticles bulk sample, all the time during

μSR measurements. The longitudinal asymmetry parameter of μSR signal $A(t)$ at a time t is defined in equation 1.

$$A(t) = [F(t) - \alpha B(t)]/[F(t) + \alpha B(t)] \quad (1)$$

where $F(t)$ and $B(t)$ are total muon events counted by the forward and backward counters, respectively, and $\alpha$ is the calibration factor reflecting the relative counting efficiencies between the forward and backward counters [12].

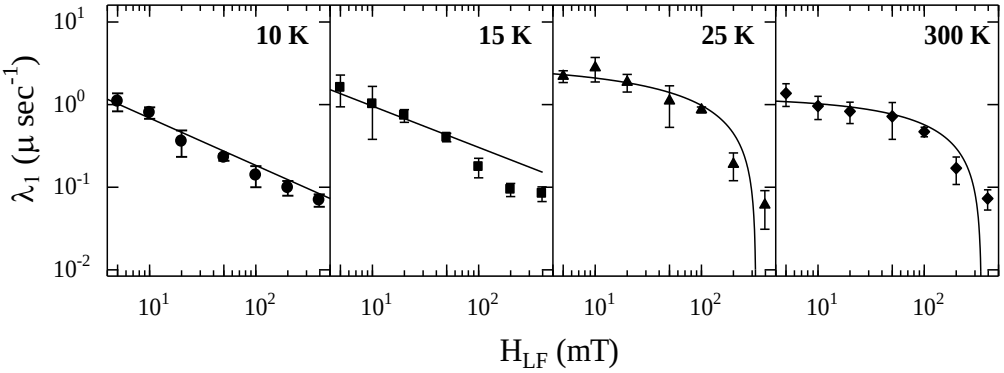


**Figure 2.** Longitudinal field dependence of $\lambda_1$ of P3HT:ZnO without light irradiation [7].

## 3. Results and Discussions

Figure 3 shows the longitudinal-field (LF) dependent variation of raw asymmetry at low temperatures of 10 K. Red circle data is asymmetry data with light irradiation and black circle data is asymmetry data without light irradiation. It is clearly shown that all initial asymmetry shifted to the higher values with increasing field due to repolarization of the muonium state [13].

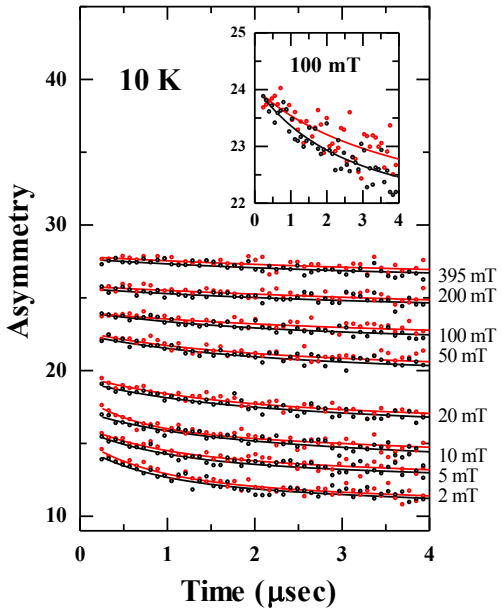


**Figure 3.** The asymmetry data of P3HT:ZnO nanoparticles at low temperatures of 10 K for various longitudinal magnetic field values (• with light irradiation and • without light irradiation).

The information of electron mobility on the polymer chain of P3HT was obtained from the spectra that were analyzed using two-component function as presented in equation 2.

$$A(t) = A_1 e^{\lambda_1 t} + A_2 e^{\lambda_2 t} \quad (2)$$

where $A_1$ and $A_2$ are the initial asymmetries, $\lambda_1$ and $\lambda_2$ are corresponding to depolarization rates associated with the fast and slow components, respectively. In figure 3, it is shown that the raw asymmetries are well fitted indicated by the solid line. It is also clearly seen that using light irradiation, the asymmetry shifted slightly as shown in the insert of figure 3. The shifting of asymmetry by light irradiation indicated the change of charge carrier transport in the samples.

The longitudinal field ($H_{LF}$) dependence of $\lambda_1$ in P3HT:ZnO is presented in figure 4. The LF dependence of $\lambda$ reflects the direction of charge diffusion in the polymer chain. That is, one-dimensional intra-chain diffusion is indicated by $\lambda$ proportional to linier field of $H^{-0.5}$ and three-dimensional inter-chain diffusion is characterized by $\lambda \sim$ C-$H^{0.5}$ curve [14]. With light irradiation, for the low temperature of 10 K, $\lambda_1$ was proportional with C-$H^{0.5}$ curve, indicating three-dimensional inter-chain diffusion. The similar tendency also observed for $H_{LF}$ dependence of $\lambda_2$. Comparing with the previous μSR data of P3HT:ZnO which the experiment was done without light irradiation, one-dimensional intra-chain diffusion is still observed in the samples at low temperature of 10 K, while three-dimensional inter-chain is observed at high temperature above 25 K [7]. With light irradiation, the crossover temperature from one-dimensional to three-dimensional of P3HT:ZnO bulk sample was obtained at lower temperature of 10 K compared to previous result at 25 K without light irradiation. This is probably related to process irradiation which initiate the production of exciton that increase number of charge carrier in sample and transport not only along the chain of polymer (one-dimensional) but also perpendicular to other chain of polymer (three-dimensional). Even though qualitatively the amount of exciton produced by light irradiation could not be determined yet, the result of μSR measurement shows that light irradiation to P3HT:ZnO effect its charge carrier transport property.

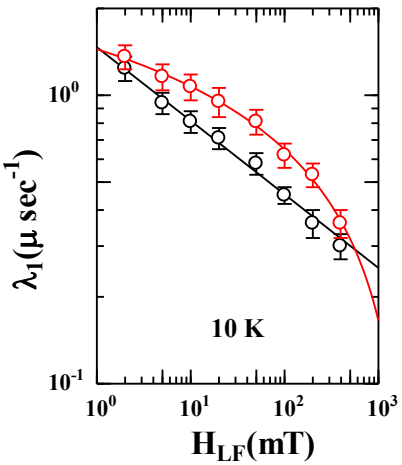


**Figure 4.** The longitudinal-field dependence $H_{LF}$ of relaxation rate $\lambda_1$ of P3HT:ZnO at low temperature of 10 K ( ○ with light irradiation and ○ without light irradiation).

## 4. Conclusions

We have studied charge carrier transport of blend P3HT and ZnO nanoparticles using muon spin relaxation method at low temperature with light irradiation. We found small changes of asymmetry for sample with and without light irradiation at low temperature of 10 K. Without light irradiation, $\lambda_1$ was proportional with $H^{-0.5}$, which indicating one-dimensional intra-chain diffusion. While with light irradiation, $\lambda_1$ was proportional with C-$H^{-0.5}$ curve which indicating three-dimensional inter-chain diffusion. With light irradiation, the charge carrier transport increased initiating by exciton production.

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