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Molecular tailoring of donor and acceptor materials of organic solar cells for improvement of their optoelectronic properties

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ABSTRACT

Improvement in the efficiency of organic solar cell (OSC) is one of the hot topics of the modern-day research. Despite environment friendliness and several other practical advantages, the power conversion efficiency (PCE) of OSC has not yet achieved the levels of the commercial inorganic solar cells. In this context, molecular tailoring of the donor and acceptor materials can help in alignment of the energy levels in order to improve PCE. In this study, we demonstrate the introduction of different functional groups on the most widely used donor and acceptor materials namely poly(3-hexylthiophene) (P3HT) and fullerene, respectively. P3HT was successfully converted into poly(4-bromo-3-hexylthiophene), poly(4-chloro-3-hexylthiophene), and poly(3-hexyl-4-nitrothiophene) through bromination, chlorination, and nitration reactions, respectively. Similarly, fullerene was converted into phenyl-C_{61}-pentanoic acid methyl ester, phenyl-C_{61}-pentanoic acid, and methyl-2-C_{61} propionate. The success of different modifications on P3HT and fullerene was monitored by ^{1}H NMR spectroscopy. Finally, the optoelectronic properties after the above-mentioned modifications were evaluated by UV–Vis spectroscopy and cyclic voltammetry.

1. Introduction

The use of nonrenewable energy sources in order to combat the energy demands of the world has increased significantly in recent times. This development has led to an increase in the global warming and environmental pollution. The substitution of nonrenewable energy sources with renewable energy sources is an alternative to hamper the rapid increase in the global warming and environmental pollution. However, the most abundant source of renewable energy, the sun, has not yet been exploited to its full potential in this regard. The conversion of solar energy into electrical energy doesn't render any noteworthy hazards to the environment [1,2]. Commercially available solar cells are based on inorganic silicon, cadmium, and cadmium sulfide materials. Their manufacturing process is associated with the release of environment polluting by-products. Organic solar cell (OSC) can be an environment friendly alternative of commercially available inorganic solar cell [2,3]. Organic semiconductor materials additionally offer several important properties such as light weight, transparency, flexibility, and easy-processability. However, the technology of OSC is still underdeveloped and its power conversion efficiency (PCE) is rather low. Two important components of any OSC are an electron donor material (conjugated polymers such as P3HT, PBDB-T-SF, and PTQ10) and an electron acceptor material (such as fullerene and ITIC). The chemical modification of these materials in order to optimize the optoelectronic properties may help to enhance the PCE [4,5].

Among the above-mentioned donor materials, polythiophenes are most widely explored owing to several associated advantages such as their low-cost, environment friendliness, thermal stability, and facile processability [6]. However, high HOMO energy level and large energy band gap are the major limitations of polythiophenes for their applications in OSC [7]. The PCE of any OSC can be improved by engineering of the donor and acceptor materials. In this context, the performance of OSC can be improved by an enhancement in the absorption efficiency of the major part of the sunlight (i.e. near Infrared radiation), by compression in the energy gap between HOMO and LUMO levels, and by down-shifting of the LUMO or up-shifting of the HOMO energy level of

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