Azido ester functionalized graphene oxide for energetic application

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Abstract

Over the previous decade, the revelation of Graphene a two-dimensional (2D) carbon structure has assembled a great deal of consideration because of its special properties, including remarkable mechanical properties, electrical, warm conductivity and so on Despite having strange properties, its low dissolvability and helpless reactivity have restricted use and made a significant test should be tended to for future application. To beat these issues. a few methodologies are investigated everywhere. Our first methodology is to orchestrate graphene oxide (GO) by the compound treatment of graphite through oxidation and further shedding in water. In light of the writing overview we have conceived functionalizing Graphene oxide with azido ester. It is referred to that when explosophore gatherings, for example, nitro, azido, and triazole are consolidated into materials, it improves the lively properties. The Graphene oxide functionalized azido-ester will be ready from esterification of Graphene Oxide (GO) by azido based liquor. For assessment of integrated items, various strategies like XRD (X-beam diffractometer), FT-IR (Fourier exchange infrared spectroscopy). TGA (Thermo-gravimetric examination), XPS (X-beam photoelectron spectroscopy), basic investigation, NMR (Nuclear attractive reverberation), SEM (Scanning electron magnifying lens) and TEM (Transmission electron magnifying lens) are utilized. We will examine the impact of it on other accessible lively composite materials by assessing fiery and mechanical properties like calorific worth, consume rate, thickness and so on and imagined fundamental upgrade.

Conjugated polymer-based bulk heterojunction (BHJ) photovoltaic effect involves the generation of a strongly bound electron-hole pair (exciton) in a p-type semiconductor under illumination and the subsequent charge collection at reverse electrodes. The charge collection therefore, requires exciton diffusion and dissociation for charge formation. This can only be achieved by creating a heterojunction interface with an electron donor (D) and an acceptor (A) having higher electron affinity (EA) but still lower ionization potential (IP) than that of the donor. In order to enhance the charge separation, Polythiophene based soluble conjugated polymers [e.g., poly(3-hexylthiophene) P3HT] and fullerene (C60) derivative [Phenyl-C61-Butyric-Acid-Methyl Ester (PCBM)] have been extensively studied as the electron donor (D) and acceptor (A). The photovoltaic devices based on this material combination are widely recognised as a low cost, roll-to-roll production on light weight flexible substrates and environment-friendly alternative for inorganic Si based devices. Solution based processability and low fabrication temperature could diminish the power utilisation cost to a large extent, serving rapid expansion photovoltaic technology implementation. in Subsequently, photovoltaic devices can be produced on the large area using screen printing, doctor blading, inkjet printing or spray deposition on plastic substrates. With momentous advances and great optimisation, conjugated polymer based photovoltaic cells have reached power conversion efficiency 5-6%.

Introduction

Although BHJ devices have numerous advantages, yet their ultimate efficiency is limited by inefficient charge transport. This may be due to curtailed trail in the random percolation network, phase-segregation, isolated domains and structural traps in the form of dead ends. Therefore, the bottleneck here is to offer continuous pathways among all components and hence, afford efficient charge transport to the opposite electrodes with minimized recombination possibility. Ago et al., Geng et al. and several other groups suggested the substitution of 0D fullerenes with 1D allotrope of carbon nanomaterials such as carbon nanotubes (CNTs), while Huynh et al. and Boucle et al. have utilised inorganic nanorods to overcome the charge-transport limitation. The high EA, ballistic carrier mobility and 1D nanostructure with large surface/interface area of CNTs are expected to reduce the structural traps and favor charge transfer. However, significant improvement in the overall device

Anshuman, Hema Singh and Shaibal Banerjee Defence Institute of Advanced Technology, India, E-mail: upadhyay.anshuman@gmail.com performance has not been achieved. The efficiency of CNTs based photovoltaic cells is rather low, usually below 0.5% due to their rough bundled surface. These bundles create an obstacle in device fabrication as they protrude up from the active layers resulting in the short circuit.

The utilization of the two-dimensional (2D) single atomic carbon sheets of graphene with remarkable electronic, thermal and mechanical properties can eliminate this problem, reducing the surface roughness to few nanometers. Graphene, among all the allotropes of carbon, is known to illustrate the highest room temperature carrier mobility ($\approx 20,000 \text{ cm} 2 \text{ v} - 1 \text{ s} - 1$). Also, due to superior electronic properties, graphene has found successful application in the photovoltaics as both the electron acceptor material and the transparent electrode by replacing the indium tin oxide (ITO) and fluorine tin oxide (FTO). In addition, it is worth mentioning that the one-atom thickness and large 2D basal plane with the huge surface area ($\approx 2600 \text{ m} 2 \text{ g} - 1$) can facilitate a larger interface in the polymer matrix for charge generation and a continuous trail for electron transfer. However, the efficiency of devices, fabricated using graphene is significantly limited in comparison to the devices fabricated using fullerene adducts. This is essentially due to its conductor character, which considerably restrains the effective hole mobility and favours the development of recombination pathways. Another drawback which precludes the wide spread use of graphene for photovoltaic is their apparent insolubility in the common organic solvent which hampers their processability.

To overcome the first drawback it has been suggested in the literature to use graphene in doping concentration in P3HT:PCBM based devices, where the graphene not only act as electron acceptors but also provide a large specific surface area at the polymer/graphene interfaces for exciton dissociation. Another drawback can be overcome by functionalization of graphene covalently or non-covalently, enhancing their solubility and thereby render them processable. Consequently, numerous functionalization methods, including grafting or noncovalent adsorption (via π - π interaction) of polymers such as poly(3-alkylthiophenes) (P3ATs), (P3HT) or poly(sodium 4-styrenesulfonate). Furthermore. asymmetrical functionalization of the graphene surface and edge with different moieties like porphyrin, (pamino)phenyl hydroquinon, 4-aminibenzoic acid (ABA), phenyl isocyanate, diazonium salts, λ -iodanes, and ionic liquid 1-butyl-3-aminopropyl imidazolium chloride, have been developed for preparing solutionprocessable graphene sheets. In addition to these, solution-generated dibromo carbene (DBC) radicals and surface-initiated atom transfer radical polymerization methods are also discussed for controlled band-gap manipulation of graphene. Graphene undergoes Diels-Alder (D-A) reactions or nitrene [2+1] cycloaddition reaction represents a promising path for selective graphene surface modification with well-defined functional groups. However, nitrene cycloaddition reaction possesses additional advantage that they introduce cyclopropane functionalities in place of the partial double of the π -conjugated structure of graphene. This cyclopropane structure has hetero-atom nitrogen (N), which can drastically disrupt the geometries and electronic state of graphene.

Conclusion

Encouraged by these reports, we have covalently functionalized graphene via the 1,3-dipolar [2+1] cycloaddition of two derivatives of aryl azide resulting in aziridine adducts on the graphene surface. To our knowledge, there have been many previous studies of nitrenes derived from perfluorophenyl azide which have found applications as photoaffinity labelling (PAL) agents and in functionalization of carbon materials like fullerene, SWCNT, and derivatizing graphene for semiconducting devices and photovoltaics. Recently, Faghani et. al. has reported one-pot nitrene [2+1] cycloaddition reaction under mild conditions using 2azido-4,6-dichloro-1,3,5-triazine with thermally reduced graphene oxide. But fluoro and chloro derivatives have many environmental issues and are tedious to synthesize due to long processing time and large amount of azide derivative used. Intended by this, for the first time, we have utilized phenvlnitrenes substituted with orthoester/anhydride groups for efficient functionalization of graphene which is not only environmental benign but can also efficiently functionalize graphene using less wt.% compared to previous report. The presence of disubstituted electron withdrawing groups enhance the lifetime of singlet nitrene resulting in the formation of aziridine bond by [2+1] cycloaddition with sp2 carbon of graphene. The presence of aziridine adducts with different functional molecules on the graphene sheets not



only provide a highly stable solution in both polar and non polar solvents but also supposed to modify the electronic structures of graphene. These aryl azide functionalized graphene (f-graphene I & II) when utilized in doping concentration (1-5 wt%) in P3HT: PCBM (1:1 blend) photovoltaic device, enhanced their power conversion efficiency (n) with respect to the P3HT:PCBM counterpart under AM 1.5 illumination (100 mW/cm2).

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