



# Poly(ethylene terephthalate): Rubbish could be low cost anode material of lithium ion battery

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## ARTICLE INFO

### Keywords:

Waste resource utilization  
Li-ion battery  
Organic anode materials  
Poly(ethylene terephthalate)  
Charge/discharge mechanism

## ABSTRACT

Tremendous poly(ethylene terephthalate) (PET) plastics has been abandoned into the environment as rubbish, which is inert and accumulated in the ecosystem across the globe. In the present work, PET plastics are changed into PET particles through a simple low temperature solvothermal treatment, which is applied as anode material of lithium ion battery. The redox peaks in the positive and negative scanning of CV (Cyclic Voltammetry) are 0.9 and 1.1 V, respectively, and the reversible capacity is about 200 mAh/g at current density of 100 mA/g. The DFT (Density Functional Theory) calculation results shows that the inserted lithium ion is coordinated with two oxygen ions, which are on the two neighboring chains, respectively, and per formula of PET ( $C_{10}H_8O_4$ ) could store two lithium ions, i.e. the theoretical capacity is 279 mAh/g. The calculated redox potential is also consistent with the experimental results. The ex situ XRD (X-ray Diffraction), FTIR (Fourier transform infrared) and XPS (X-ray photoelectron spectroscopy) measurement results in the charge/discharge are consistent with DFT calculation results, and confirm that demonstrate that the polymer's lithiation/delithiation process is reversible. The present work provides a novel way to utilize the PET plastics waste.

**Significance:** Innumerable PET plastics have been abandoned, which is resistance to natural degradation. Here the PET plastics were transformed into PET particles after a solvothermal treatment, of which the size was in the range from several microns to tens of microns. The PET particles were tested as the anode material of Lithium ion battery, and its reversible capacity is about 200 mAh/g at 100 mA/g. The energy storage mechanism is attributed to redox reaction between the inserted lithium ions and the ester groups on PET chain, which is confirmed through the DFT calculation and XRD, FTIR and XPS measurement results. This is the first report for PET plastics used as electrode materials, and it provides a new way to utilize the PET refuse.

## 1. Introduction

Plastics have special properties such as plasticity, durability, transparency, low weight and so on, which have been produced in large scale > 100 years [1]. Most of plastic products are persistent in natural environment due to that the plastic constituent is very difficult to be biologically degraded. Particularly, poly(ethylene terephthalate) (PET) containing aromatic components, is chemically inert, and resistance to natural degradation [2–3]. Recently, > 50 million tons of PET is produced per year, which is widely used in clothing fibers, liquids or foods' containers, and **thermoforming** for manufacturing, etc. [4]. Until now, a tremendous amount of PET has been released into the environment, which is accumulated in the ecosystems across the globe. Recently, some works have been reported for the biodegradation of PET with bacterium [5]. Is it possible to explore a way to utilize the PET rubbish as a useful resource is urgent.

Organic compounds have received great attention as active electrode materials of rechargeable batteries due to their structural diversity, environment friendliness, renewability, and low cost, etc. [6–11]. Various types of organic compounds, such as conjugated amine [12–13], conjugated hydrocarbon [14–15], conjugated carbonyl [16–19], conjugated thioether [20–21], nitroxylradical [22–23], and organodisulfide [24–25], have been reported for high electrochemical performance as electrode material of lithium/sodium ion battery. However, there are very few reports for organic electrode materials directly gained from household waste or industrial refuse. PET has typical conjugated structure, and two ester groups are in per formula. Is it possible to make use of PET refuse as organic electrode material of lithium ion battery? Until now, no work is reported on that.

In the present work, PET powder is prepared from PET plastics through a simple low temperature solvothermal treatment (about 110 °C), which could be used as anode material of lithium ion battery.

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The XRD and FTIR results demonstrate that the product is still PET, which is not decomposed into its monomers, terephthalic acid (TPA) and ethylene glycol (EG). For PET, two lithium ions could be stored in per formula ( $C_{10}H_8O_4$ ), and the theoretical capacity is about 279 mAh/g. The redox peaks in the positive and negative scanning of CV are 0.9 and 1.1 V, respectively. The reversible capacity is 150 mAh/g at the charge/discharge current of 100 mA/g, which is close to the theoretical value. The ex situ XRD, FTIR and XPS experimental results demonstrate that the lithiation/delithiation process is reversible and the polymer's crystal structure keeps stable during the process. Subsequently, the DFT calculation results discover that the inserted lithium ion stays between two neighboring PET chains and is coordinated with two oxygen ions of the two chains, which is consistent with the XRD, FTIR and XPS results, and the calculated redox potential agrees with the measured value in CV testing.

## 2. Experimental and theoretical calculation method

The raw material of PET plastic was obtained from a bottle produced with PET. Other chemicals, NMP (*N*-methyl-2-pyrrolidone) and  $Zn(NO_3)_2 \cdot 6H_2O$  (both purchased from Fuchen Limited, China) were used as received. The PET powder was produced through a simple solvothermal method. Initially, 3.0 g of  $Zn(NO_3)_2 \cdot 6H_2O$  was dissolved in 50 mL NMP under constant stirring. The bottle was cut into small pieces, and 2.0 g of them were added to the Zinc nitrate solution. The resulting solution was transferred into a 50 mL Teflon-lined autoclave, and the autoclave was capped tightly and placed in an oven at 120 °C for 12 h. After cooling down to room temperature in fumehood, the light yellow product was obtained by removing the mother liquor, and washed with ethanol. Finally, the product was dried at 100 °C for 12 h in vacuum oven. The process is presented in Scheme 1.

As-synthesized PET powder and PET electrodes at different states of charge were analyzed by X-ray Diffraction (XRD) in the  $2\theta$  range 10°–50° at a scanning rate of 1° min<sup>-1</sup> by an X-ray diffractometer (Bruker D8 Advance) with a Cu-K $\alpha$  radiation at 40 kV and 40 mA. Scanning electron microscopy (SEM) images were taken on a scanning electron microscope (Hitachi, S-4300). Thermo gravimetric analysis (TGA) was performed by a TG-DTA instrument (Seiko Instruments, 6300). The sample was heated from 25 to 600 °C in N<sub>2</sub> at a rate of 10 °C min<sup>-1</sup>. XPS analysis of the PET electrodes at different states of discharged and charge, were performed on an Axis Ultra (Kratos Analytical Ltd.).

In electrochemical characterization of the electrodes, CR2032 coin cells were assembled in an argon-filled glove box, where both the moisture and oxygen contents were < 0.5 ppm. For fabrication of the working electrodes, PET, acetylene black, binder (polyvinylidene fluoride) were homogeneously mixed in a weight ratio of 7:2:1 in *N*-methyl-2-pyrrolidone (NMP) to form a slurry. The slurry was then coated on a 15  $\mu$ m thick copper foil with mass loading of 1.5–2 mg/cm<sup>2</sup>. Pure lithium foil (Aldrich) was used as the counter electrode, and the electrolyte was 1 M LiPF<sub>6</sub> in a 50:50 w/w mixture of ethylene carbonate and diethylcarbonate. A battery tester (Neware, Shenzhen, China) was used to conduct the galvanostatic measurements. Cyclic Voltammetry (CV) experiments were performed using a potentiostat (VMP3, BioLogics, France).

The DFT (Density Functional Theory) has been widely applied in the field of lithium ion battery, such as predicting the potential of the electrode material, calculating the migration barrier of lithium ion and simulating the dynamics of the charge/discharge process [26]. In the present work, the theoretical calculations were performed using the Vienna Ab initio Simulation Package (VASP) [27] within the projector augmented-wave (PAW) [28] method. The exchange-correlation potential between electrons is described with the generalized gradient approximation (GGA) with the functional parameterization of PBE [29], and the long-range van der Waals interaction between organic molecule is calculated with the dispersion-corrected Density Functional



Scheme 1. The process to produce active PET particles.

Theory, DFT-D2 [30].  $5 \times 3 \times 2$  k-Point is sampled in the first Brillouin zone. The energy cutoff of plane wave is set up to 400 eV.

The intercalation potentials were obtained by the total energy between the lithiated state and the delithiated state, and it is calculated with the following equation [31]:

$$V = -\frac{E_{Li_nPET} - E_{PET} - nE_{Li}}{nF}$$

where  $n$  is the number of inserted Li-ions, and here its value is 2;  $F$  is the Faraday constant. Each total energy calculation is based on the completely optimized crystal structure  $\varphi_{Li}$ .

## 3. Results and discussion

The PET plastic bottles, as shown in Fig. 1a, were changed into small particles through scissoring and solvothermal treatments (the process is shown in Scheme 1). In the SEM image (Fig. 1b), the size of prepared PET particles ranges from several microns to tens of microns, which have irregular shapes. The XRD profile of prepared PET is the same as that of the commercial powder purchased from Shenghao plastic materials Limited (the commercial particles are larger than 1 mm, which could be directly distinguished by eyes), as shown in Fig. 1c, and is indexed in the spacegroup *P*-1 as the crystal structure previously reported by Fu et al. [32] The four main broad peaks, (01–1), (010), [1–10] and (100) imply the low crystallinity, which is common for polymer materials.

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