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Novel cobalt-incorporated two dimensional covalent organic frameworks for supercapacitor applications

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ABSTRACT

Covalent-organic frameworks (COFs), are a promising new class of crystalline porous organic materials with confined structures either in 2D or 3D domains. The current study focuses on using a solvothermal approach consisting of sealed pyrex tubes to synthesize two-dimensional TBP-COF and TBP-COF that have been doped with cobalt (Co) (TBP-Co@COF). The results of the experimentally acquired X-ray diffraction study were compared with those from simulations, and it was discovered that both are in good agreement. A thorough theoretical analysis of the layer packing in AA stacking (P1) and AB stacking (P1) modes using the Materials Studio revealed that AA stacking is more stable than the AB stacking (P1) structure. The formation of imine linkage and incorporation of Co into the COF are indicated by the result of XPS. Unaggregated dispersion of Co particles can be seen on the square and rectangular sheets of TBP-COF in TEM and SEM images. Both materials are fabricated as electrode materials and evaluated for their supercapacitor applications. The TBP-Co@COF shows an enhanced specific capacitance (CSp) of 975F/g compared to the TBP-COF (827F/g) at 2 mV/s scan rate. TBP-Co@COF exhibit an energy density (ED) of 69 Wh/kg even at a high power density (PD) of 75000 W/kg and also retains 79 % of its initial capacitance up to 2000 cycles. TBP-COF and TBP-Co@COF were fabricated for an asymmetric supercapacitor device (ASD) and found to exhibit a CSp of 191F/g at a scan rate of 2 mV/s.

1. Introduction

The pursuit of renewable energy sources is essential for achieving a sustainable economy in the future [1,2]. Traditional renewable energy sources like wind, sun, and hydropower are sporadic in nature. So any system using renewable energy must include an energy storage component [3]. A type of energy storage system that is frequently employed nowadays is supercapacitors (SCs) [4,5]. Supercapacitors are high-power energy storage and delivery systems that have a rapid rate of energy delivery. They are excellent for uses like electric vehicle acceleration, uninterruptible power supply (UPS), openers in aircraft, emergency doors, and granty cranes due to their capacity to produce higher power densities [6–8].

Due to their customizable interlayer spacing, 2D materials have recently attracted a lot of attention for electrochemical energy storage applications, due to their property to host and transport charge carriers [9–11]. These 2D materials have a large surface area to promote more favorable interactions at the electrode–electrolyte interface. One of the first and most extensively researched 2D materials for energy storage applications is graphene [12–14]. In graphene-based electrodes, the occurrence of individual layer re-stacking can lead to constrictive problems such as poor electrolyte transport and reduced ionic mobility, thus lowering the electrochemical charge storage performance [15,16]. It has been discovered that adding pores or holes to 2D layers can effectively increase the charge storage capacity of graphene in supercapacitors [17,18]. In this way, making new 2D organic graphene analogs with precise porosity and redox abilities that can be controlled can be very helpful for storing electrochemical energy effectively [10–23].

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