



Full Length Article

Porous carbon materials based on biomass for acetone adsorption: Effect of surface chemistry and porous structure

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ABSTRACT

The relative influence of porous structure and functional groups of porous carbon materials for acetone adsorption is presented in this article. Here, we have successfully prepared oxygen and nitrogen doping porous carbons (ONPCs) by a hydrothermal method using waste tobacco stem as the carbon precursor and ethylenediamine as a nitrogen source. The resulting ONPCs have high specific surface (906–2940 m² g⁻¹) and chemical compositions (1.80–5.22% N and 5.81–11.77% O). This carbon shows high acetone adsorption capacity (*i.e.*, 16.91 mmol g⁻¹ at 25 °C and 18 kPa). The pore volume and specific surface area of ONPCs were found to be determinative factors for acetone adsorption at high pressure, and the introduction of oxygen and nitrogen into carbon surface can improve acetone adsorption at low pressure. Molecular simulations results suggest that adsorption capacity of acetone is improved at low pressure after doping of oxygen and nitrogen functional groups, but equilibrium adsorption capacity is unchanged. This is in good agreement with the experimental results that these functional groups are primarily responsible for the materials' low-pressure acetone adsorption capacity. This work provides insights into material design and further development for acetone adsorption.

1. Introduction

Enforcing strict environmental regulations is already the industry looking for better ways to control the emission of various pollutants, including volatile organic compounds (VOCs) in exhaust gases [1,2]. The concentration of VOCs in the air is generally in the range of 50–2000 ppm and many methods have been taken to help reduce industrial-scale gaseous VOCs emissions including: catalysis, absorption and condensation methods [3–5]. Among these methods, the adsorption technology has been believed as an effective technology for trace amount VOCs uptake and separation from contaminated air in the outdoor environment [5]. Generally, activated carbons have positive features on large pore volume, high specific surface area and chemistry stability, they are therefore used as the adsorbents for removal VOCs by adsorption [6].

Fundamentally, the structure properties and surface chemistry provide an effective way to enhance the VOCs adsorption performance [7]. Previous investigates have shown that the acetone adsorption performance depends on the high specific surface area of carbon, because the surface area provides the adsorption sites during the adsorption process [8,9]. For instance, Das et al. [10] compared the interaction between toluene adsorption and specific surface area, and

found that toluene breakthrough time in ACF of larger surface area (1700 m² g⁻¹) was four times that of smaller surface area (1000 m² g⁻¹). It has been pointed out that micropores, especially narrow micropores, control the VOCs adsorption on porous carbon. Lillo-Ródenas et al. [11] indicated the impact of pore size distribution on adsorption of VOCs. It has been reported that after removal of the oxygen functional groups by thermal treatment, the pore size (size < 0.7) volume of AC directly determines the adsorption capacity of benzene rather than the total micropore volume. In addition to the structure properties, surface chemistry of carbon materials may also play an important role in VOCs adsorption [12]. The surface chemistry of carbon materials is determined by heteroatoms on their surface functional groups. The heteroatoms primarily include oxygen, nitrogen, sulfur and phosphorus etc., among them, the oxygen and nitrogen functional groups have beneficial effect on the adsorption. Numerous the oxygen groups are the source of acidity on the carbon surface, which beneficial to the hydrophilic VOCs adsorption [13,14]. For instance, Dimotakis [15] and Kwon [16] had shown that the oxygen groups can improve acetone adsorption performance due to dipole-dipole and hydrogen bonds interactions between acetone molecules and functional groups. In addition, the present of nitrogen groups promotes polar interactions between carbon surface and acetone molecules. Li

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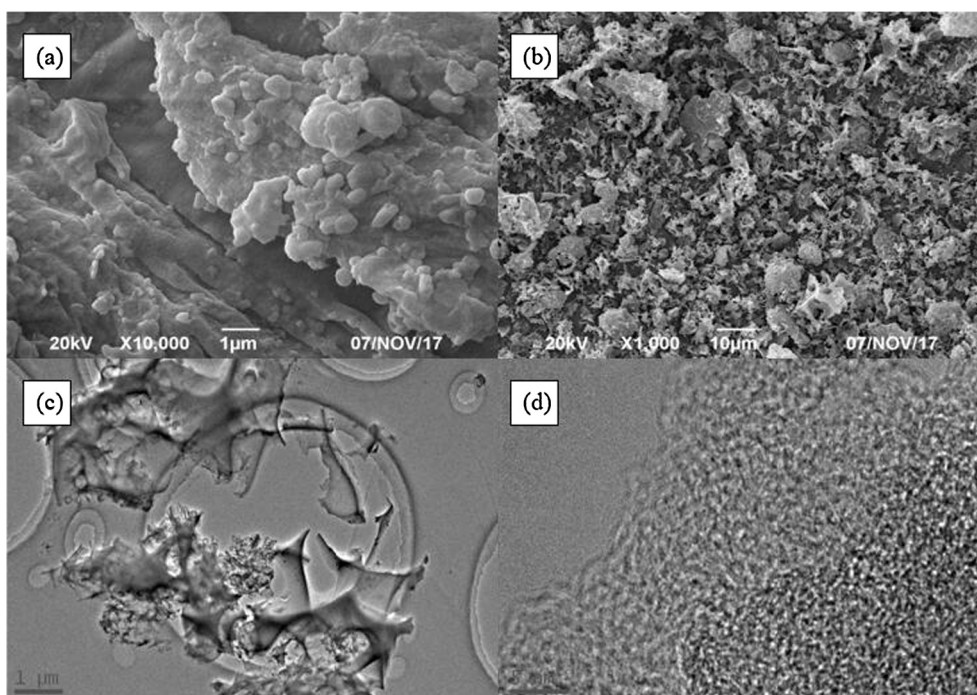


Fig. 1. SEM images of tobacco stem hydrochar (a) and porous carbon derived from tobacco stem (b). TEM images of ONPC600 (c) and (d).

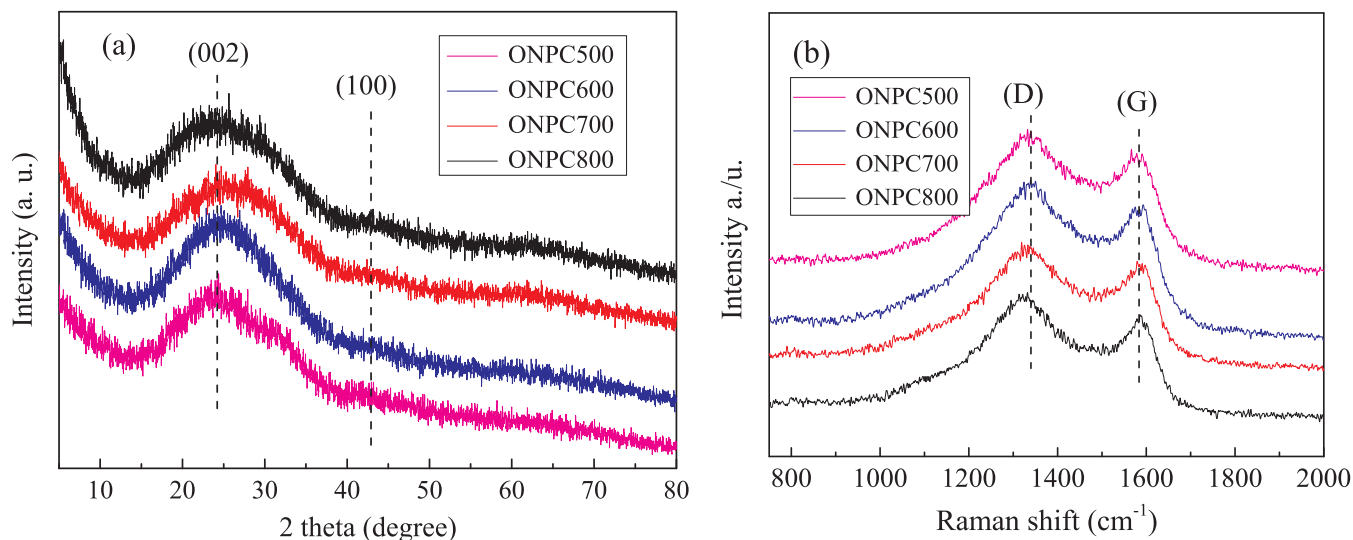


Fig. 2. X-ray diffraction (XRD) (a), and Raman spectra (b) of ONPC samples.

[17] had reported that N-doped porous carbon by modification with NH_3 for increasing the surface polarity and improved acetone adsorption capacity.

In this work, we have successfully prepared N, O-doped porous carbon materials by two simple steps: (i) Hydrothermal treatment with waste tobacco stem as the carbon precursor and ethylenediamine as the nitrogen source; and (ii) activated using KOH as an activation agent. It is found that the carbonization temperature affected the porous structure, doping conditions, and the adsorption of acetone. More importantly, the large pore volume can offer superior acetone adsorption capacity at high pressure and the introduction of oxygen and nitrogen into carbon surface can improve acetone adsorption at low pressure. The grand canonical Monte Carlo (GCMC) method is used to simulate acetone adsorption in carbon slit pore model. The results show that the functional groups can improve acetone adsorption capacity at low pressure, however, the equilibrium adsorption capacity is unchanged.

2. Experimental section

2.1. Preparation of porous carbon

In a typical synthesis, 8 g tobacco stem and 4 mL ethylenediamine were added into a 100 mL Teflon-lined stainless autoclave. Hydrothermal reaction was conducted at 180 °C for 10 h. The obtained samples were filtered, washed with distilled water and dried at 120 °C. The dried powders were combined with KOH at the weight ratio of 2. The mixture was then carbonized in a tubular furnace for 1 h under a nitrogen atmosphere. The target temperature and heating rate were 500–800 °C and 3 °C min⁻¹, respectively. The resulting samples were then thoroughly washed with 5% HCl solution to remove any inorganic salts and distilled water until neutral PH was reached. The samples were denoted as ONPCx, where x (x = 500, 600, 700, or 800) is the activating temperature.

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